

Title:

**Analytical Detection and Quantification of
Energetic Materials
A Literature Review**

Author(s):

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Analytical Detection and Quantification of Energetic Materials
A Literature Review
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Executive Summary

Nearly all, if not all, known analytical chemical methods have been investigated for their applicability to the detection of explosive materials. The methods can be subdivided into those that detect vapors or particles emitted from the materials, those that detect dissolved or suspended solids in solutions, and those that probe solid materials. Vapor or particle detection systems are best suited for personnel monitoring, such as in portals, but none of the methods investigated to date solves the simultaneous problems of speed, sensitivity, and selectivity required for e.g., passenger screening. A wide variety of very sensitive methods have been developed for environmental analysis of explosives and/or their degradation products, where the speed requirement is much relaxed. The most difficult area of research and development is for tools that probe solid objects to locate concealed explosives. Mostly nuclear methods have been used, but recent advances in millimeter wave and terahertz imaging may provide a more society acceptable alternative.

The greatest difficulty with all methods to date is the small subset of the list of explosive materials that have been used in their development or characterization. There should be a concerted effort to expand the number of materials studied.

The references are given in each section in reverse chronological order, unless the concept narrative dictated otherwise.

The section on implementation of detection systems is composed of material extracted from various Internet sources as of January 2003 and information and statistics obtained from FAA and National Academy reports.

1 List of explosive materials [from ATF P 5400.8 (4/2002)]

Acetylides of heavy metals.
Aluminum containing polymeric propellant.
Aluminum ophorite explosive.
Amatex.
Amatol.
Ammonal.
Ammonium nitrate explosive mixtures (cap sensitive).
Ammonium nitrate explosive mixtures (non-cap sensitive). (Blasting agent)
Ammonium perchlorate composite propellant.
Ammonium perchlorate explosive mixtures.
Ammonium picrate [picrate of ammonia, Explosive D]
Ammonium salt lattice with isomorphously substituted inorganic salts.
ANFO [ammonium nitrate-fuel oil]. (Blasting agent)
Aromatic nitro-compound explosive mixtures.
Azide explosives.

Baranol.
Baratol.
BEAF [1, 2-bis (2, 2-difluoro-2- nitroacetoxyethane]
Black powder.
Black powder based explosive mixtures.
Blasting agents, nitro-carbo-nitrates including non-cap sensitive slurry and water gel explosives.
Blasting caps.
Blasting gelatin.
Blasting powder.
BTNEC [bis (trinitroethyl) carbonate]
BTNEN [bis (trinitroethyl) nitramine]
BTTN [1,2,4 butanetriol trinitrate]
Bulk salutes.
Butyl tetryl.

Calcium nitrate explosive mixture.
Cellulose hexantrate explosive mixture.
Chlorate explosive mixtures.
Composition A and variations.
Composition B and variations.
Composition C and variations.
Copper acetylide.
Cyanuric triazide.
Cyclonite [RDX].
Cyclotetramethylenetetranitramine [HMX]
Cyclotol.
Cyclotrimethylenetrinitramine [RDX]

DATB [diaminotrinitrobenzene]
DDNP [diazodinitrophenol]
DEGDN [diethyleneglycol dinitrate]
Detonating cord.
Detonators.
Dimethylol dimethyl methane dinitrate composition.
Dinitroethyleneurea.
Dinitroglycerine [glycerol dinitrate]
Dinitrophenol.
Dinitrophenolates.
Dinitrophenyl hydrazine.
Dinitroresorcinol.
Dinitrotoluene-sodium nitrate explosive mixtures.
DIPAM [dipicramide; diaminohexanitrobiphenyl]
Dipicryl sulfone.
Dipicrylamine.
Display fireworks.
DNPA [2,2-dinitropropyl acrylate]
DNPD [dinitropentano nitrile]
Dynamite.

EDDN [ethylene diamine dinitrate]
EDNA [ethylenedinitramine]
Ednatol
EDNP [ethyl 4.4-dinitropentanoate]
EGDN [ethylene glycol dinitrate]
Erythritol tetranitrate explosives.
Esters of nitro-substituted alcohols.
Ethyl-tetryl.
Explosive conitrates.
Explosive gelatins.
Explosive liquids.
Explosive mixtures containing oxygen-releasing inorganic salts and hydrocarbons.
Explosive mixtures containing oxygen-releasing inorganic salts and nitrobodies.
Explosive mixtures containing oxygen-releasing inorganic salts and water insoluble fuels.
Explosive mixtures containing oxygen-releasing inorganic salts and water soluble fuels.
Explosive mixtures containing sensitized nitromethane.
Explosive mixtures containing tetranitromethane (nitroform).
Explosive nitro compounds of aromatic hydrocarbons.
Explosive organic nitrate mixtures.
Explosive powders.

Flash powder.
Fulminate of mercury.
Fulminate of silver.
Fulminating gold.

Fulminating mercury.
Fulminating platinum.
Fulminating silver.

Gelatinized nitrocellulose.
Gem-dinitro aliphatic explosive mixtures.
Guanyl nitrosamino guanyl tetrazene.
Guanyl nitrosamino guanylidene hydrazine.
Guncotton.

Heavy metal azides.
Hexanite.
Hexanitrodiphenylamine.
Hexanitrostilbene.
Hexogen [RDX]
Hexogene or octogene and a nitrated N-methylaniline.
Hexolites.
HMTD [hexamethylenetriperoxidediamine]
HMX [cyclo-1,3,5,7-tetramethylene 2,4,6,8-tetranitramine; Octogen]
Hydrazinium nitrate/hydrazine/aluminum explosive system.
Hydrazoic acid.

Igniter cord.
Igniters.
Initiating tube systems.

KDNBF [potassium dinitrobenzo-furoxane].

Lead azide.
Lead mannite.
Lead mononitroresorcinate.
Lead picrate.
Lead salts, explosive.
Lead styphnate [styphnate of lead, lead trinitroresorcinate]
Liquid nitrated polyol and trimethylolethane.
Liquid oxygen explosives.

Magnesium ophorite explosives.
Mannitol hexanitrate.
MDNP [methyl 4,4-dinitropentanoate].
MEAN [monoethanolamine nitrate].
Mercuric fulminate.
Mercury oxalate.
Mercury tartrate.
Metriol trinitrate.
Minol-2 [40% TNT, 40% ammonium nitrate, 20% aluminum].

MMAN [monomethylamine nitrate]; methylamine nitrate.

Mononitrotoluene-nitroglycerin mixture.

Monopropellants.

NIBTN [nitroisobutametrial trinitrate].

Nitrate explosive mixtures.

Nitrate sensitized with gelled nitroparaffin.

Nitrated carbohydrate explosive.

Nitrated glucoside explosive.

Nitrated polyhydric alcohol explosives.

Nitric acid and a nitro aromatic compound explosive.

Nitric acid and carboxylic fuel explosive.

Nitric acid explosive mixtures.

Nitro aromatic explosive mixtures.

Nitro compounds of furane explosive mixtures.

Nitrocellulose explosive.

Nitroderivative of urea explosive mixture.

Nitrogelatin explosive.

Nitrogen trichloride.

Nitrogen tri-iodide.

Nitroglycerine [NG, RNG, nitro, glyceryl trinitrate, trinitroglycerine].

Nitroglycide.

Nitroglycol [ethylene glycol dinitrate, EGDN].

Nitroguanidine explosives.

Nitronium perchlorate propellant mixtures.

Nitroparaffins Explosive Grade and ammonium nitrate mixtures.

Nitrostarch.

Nitro-substituted carboxylic acids.

Nitrourea.

Octogen [HMX]

Octol [75 percent HMX, 25 percent TNT].

Organic amine nitrates.

Organic nitramines.

PBX [plastic bonded explosives].

Pellet powder.

Penthrinite composition.

Pentolite.

Perchlorate explosive mixtures.

Peroxide based explosive mixtures.

PETN [nitropentaerythrite, pentaerythrite tetranitrate, pentaerythritol tetranitrate].

Picramic acid and its salts.

Picramide.

Picrate explosives.

Picrate of potassium explosive mixtures.

Picratol.

Picric acid (manufactured as an explosive)

Picryl chloride.

Picryl fluoride.

PLX [95% nitromethane, 5% ethylenediamine]

Polynitro aliphatic compounds.

Polyolpolynitrate-nitrocellulose explosive gels.

Potassium chlorate and lead sulfocyanate explosive.

Potassium nitrate explosive mixtures.

Potassium nitroaminotetrazole.

Pyrotechnic compositions.

PYX [2,6-bis(picrylamino)-3,5-dinitropyridine]

RDX [cyclonite, hexogen, T4, cyclo-1,3,5,-trinlethylene-2,4,6,-trinitramine; hexahydro-1,3,5-trinitro-S-triazine]

Safety fuse.

Salts of organic amino sulfonic acid explosive mixture.

Salutes (bulk).

Silver acetylide.

Silver azide.

Silver fulminate.

Silver oxalate explosive mixtures.

Silver styphnate.

Silver tartrate explosive mixtures.

Silver tetrazene.

Slurried explosive mixtures of water, inorganic oxidizing salt, gelling agent, fuel, and sensitizer (cap sensitive).

Smokeless powder.

Sodatol.

Sodium amatol.

Sodium azide explosive mixture.

Sodium dinitro-ortho-cresolate.

Sodium nitrate explosive mixtures.

Sodium nitrate-potassium nitrate explosive mixture.

Sodium picramate.

Special fireworks.

Squibs.

Styphnic acid explosives.

Tacot [tetranifro-2,3,5,6-dibenzo- 1,3a,4,6a tetrazapentalene].

TATB [triaminotrinitrobenzene].

TATP [triacetonetriperoxide].

TEGDN [triethylene glycol dinitrate]

Tetranitrocarbazole.

Tetrazene [tetracene, tetrazine, 1(5-tetrazolyl)-4-guanyl tetrazene hydrate].

Tetryl [2,4,6 tetranitro-N-methylaniline].

Tetrytol.

Thickened inorganic oxidizer salt slurried explosive mixture.

TMETN [trimethylolethane trinitrate]

TNEF [trinitroethyl formal].

TNEOC [trinitroethylorthocarbonate].

TNEOF Etrinitroethylorthoformate].

TNT [trinitrotoluene, trotyl, trilit, triton].

Torpex.

Tridite.

Trimethylol ethyl methane trinitrate composition.

Trimethylolthane trinitrate- nitrocellulose.

Trimonite.

Trinitroanisole.

Trinitrobenzene.

Trinitrobenzoic acid.

Trinitrocresol.

Trinitro-meta-cresol.

Trinitronaphthalene.

Trinitrophenetol.

Trinitrophloroglucinol.

Trinitroresorcinol

Tritonal.

Urea nitrate

Water-bearing explosives having salts of oxidizing acids and nitrogen bases, sulfates, or sulfamates (cap sensitive)

Water-in-oil emulsion explosive compositions

Xanthamones hydrophilic colloid explosive mixture.

1.1 Classes of explosives:

Military explosives (e.g., amatol, ammonal, Comp A-3, Comp B, Comp C-4, Cyclotol, DBX, Detasheet, H-6, HBX-1, hexal, LX-10, LX-17, octol, PBX-9404, PBX-9501, PBXN-107, PE 4, pentolite, picratol, PTX-1, PTX-2, Semtex-H, tetrytol, torpex, trigonol, tritonal)

Dynamites

Ammonium nitrate based explosives

Slurry and emulsion explosives

Propellants

Special purpose explosives (detonation cord, blasting caps, primers)

2 Detection methods

First, it must be noted that the above list of ATF recognized explosives contains nearly 250 materials, yet nearly all detection methods have been developed and tested against a small subset, usually TNT, RDX, HMX, TATB, PETN, NG, ANFO and perhaps a few other common materials, impurities, or decomposition products. This shortcoming is a serious flaw that needs considerable R&D to remedy. The lack of standard reference materials containing more than the usual explosive components contributes to this shortcoming. Accustandards (www.accustandard.com) has several reference material solutions available (at 0.1 and 1 mg/mL concentrations), but they only contain a variety of amino nitrotoluenes and nitrobenzenes plus RDX, HMX, and tetryl (up to 14 components). Still, the availability of any reference materials or solutions is a great improvement that has occurred in just the past few years and will help future method development and qualification efforts.

There have been many reviews of the explosive detection literature in the recent past. References to those articles follow:

1. Urbansky ET, 2000. Quantitation of perchlorate ion: Practices and advances applied to the analysis of common matrices. *Crit. Rev. Anal. Chem.* 30: 311-343
2. Yinon J, *Forensic and Environmental Detection of Explosives*, Wiley, Chichester, 1999
3. Steinfeld JJ, Wormhoudt J, *Ann. Rev. Phys. Chem.* 1998, 49:203-32
4. Committee on Commercial Aviation Security. 1997. *Second Interim Rep. Fed. Aviat. Admin. Tech. Cent.*, DOT/FAA/AR-97/57
5. Fischetti M. 1997. *Technol. Rev.* 100:39-46
6. Kolla P. 1997. *Angew. Chem. Int. Ed. Engl.* 36:800-11
7. Makky WH, ed. 1996. *Proc. Explosives Detection Technology Symp. Aviation Security Technology Conf., 2nd*, Atlantic City: FAA
8. Midkiff CR, Tontarski RE Jr. 1995. *Detection and Characterization of Explosives and Explosive Residues—A Review*, *Int. ICPO-INTERPOL Forensic Sci. Symp., 11th*, Lyons
9. Oxley JC. 1995. *SPIE Proc.* 2511:217-26
10. Rouhi AM. 1995. *Chem. Eng. News* 73:10-19
11. Vourvopoulos G. 1994. *Chem. Ind.*, 297-300
12. Fainberg A. 1992. *Science* 255:1531-37
13. Yinon J, ed. 1992. *Proc. Int. Symp. Anal. Detect. Explos., 4th*, London. Dordrecht: Kluwer
14. Yinon J, Zitrin S. 1993. *Modern Methods and Applications in Analysis of Explosives*. Chichester: Wiley
15. Nyden MR. 1990. *A Technical Assessment of Portable Explosives Vapor Detection Devices*. *NIJ Rep.* 300-89. Gaithersburg, MD: NIST
16. Yinon J. 1977. *Crit. Rev. Anal. Chem.* 7:1-35

2.1 Vapor detection

Explosives have a variety of vapor pressures at room temperature, from reasonable (torr level from EGDN) through microtorr, as from TNT or DNT, to sub-nanotorr, as from HMX, making their detection via vapor methods potentially extremely difficult and material dependent. Most vapor detection methods have been demonstrated for materials with relatively high vapor pressures, such as TNT and DNT, or with heating, where decomposition is usually problematic. Vapor detection can be thwarted by sealing, packaging, or containerizing. Kolla estimates that the effective vapor pressure can be reduced by a factor of 1000 by sealing in plastics. Davidson et al. state that only the highest vapor pressure explosives can be detected under real world conditions because of the attenuation of vapors by packaging.

Interferences leading to false alarms are a difficulty with all of the techniques, either because of the inherent lack of selectivity (i.e., ability to differentiate between substances) or because the technique actually detects an additive or impurity, which could also come from sources other than explosives, such as solvents, plastics, etc. However, few studies have attempted to quantify false alarm rates in real world scenarios (see Davidson and Kolla references below). This is another area that requires a large amount of attention.

Applicable References:

17. Kolla P. 1995. *Anal. Chem.* 67(5):184A–89A
18. Davidson WR, Stott WR, Sleeman R, Akery AK. 1994. *SPIE Proc.* 2092:108–19

2.1.1 Trained animals

Concept

The canine nose is an extremely sensitive molecular sniffer, able to detect vapors at concentrations three to five orders of magnitude lower than those discernable by people. Dogs are also trainable to a specific action when a given material is detected. They are usually trained on specific substances rather than specific products.

There are problems with use of trained dogs as detectors. They fatigue, their capabilities decline with time, and they suffer from changeable moods and show behavior variations.

Other animals, such as rats, have also been studied, but the training and reliability are questionable for reliable detection.

Demonstrated materials with associated detection limits and matrix effects

No quantification found in the literature

Applicable References

19. Furton KG, Lawrence J, Myers LJ, 2001. *Talanta* 54 : 487–500

20. Williams, M., Johnston, J. M., Waggoner, L. P., Jackson, J., Jones, M., Boussom, T., Hallowell, S. F. and Petrousky, J. A. Determination of the canine detection signature for NG smokeless powder. *Second Explosives Detection Technology Symposium & Aviation Security Technology Conference*, Atlantic City, NJ, 1996, pp. 328-339.
21. Biederman, G. B. Vapor preconcentration in the detection of explosives by animals in an automated setting. In: Yinon J. (ed.), *Advances in Analysis and Detection of Explosives*, Kluwer Academic Publishers, Dordrecht, 1993, pp. 463-472.
22. Luescher, U. A. Animal behavior case of the month. *Journal of the American Veterinary Medical Association*, 1993, 203, 1538-1539.
23. Lovett, S. Explosive search dogs. *First International Symposium on Explosive Detection Technology*, Atlantic City, NJ, 1991, pp. 774-775.
24. Ternes, J. W. Integration of the human, canine, machine interface for explosives detection. *First International Symposium on Explosive Detection Technology*, Atlantic City, NJ, 1991, pp. 891-902.
25. Weinstein, S., Drozdenko, R. and Weinstein, C. Detection of extremely low concentrations of ultra pure TNT by rat. *Third International Symposium on Analysis and Detection of Explosives*, Mannheim-Neuostheim, Germany, 1989, pp. **32.31-32.34**.
26. Wright, R. H. *The Sense of Smell*, CRC Press, Boca Raton, 1982, p. 236.

2.1.2. Sampling and pre-concentration

Concept

Because vapor pressures are very low for most explosive materials, vapors are usually concentrated in some manner to improve ultimate volume detection limits. Explosives have been found to adhere to a variety of materials such as Teflon, glass, quartz, nickel, stainless steel, gold, platinum, copper, fused silica, aluminum, and plastic. A typical concentration scenario is to volume flow through a fine mesh, membrane, ribbon, or long tube of the material at room temperature, followed by flash heating to a higher temperature (ca. 150 °C) and injection of the smaller trapped volume into the analytical detection system. Several coating materials with larger trapping efficiencies (such as solid phase extraction (SPE) or gas chromatographic polymers, and even fullerenes) have been tested to decrease the collection time needed for a given detection limit.

The other concept on sampling is to collect particles by vacuuming or otherwise sweeping a volume, because the particles either have already done the task of pre-concentration, or are explosive particles themselves, leading to much easier detection. The task of collecting particulates is often performed using portals.

Surfaces of potentially contaminated objects can be swiped and the swipe analyzed in a separate step. Sometimes portals also double as swiping devices, such as the designs of Wendel and McGann et al.

There have also been efforts to develop species selective coatings for pre-concentrators, so that a separation step is included in the sample collection. (see e.g., Houser et al.). These have been coupled to a SAW device (see Gas Chromatography below) for direct detection of specific

species. coated device.

Demonstrated materials with associated detection limits and matrix effects

The adsorption efficiency can be affected by ambient temperature, so that detection limits based on collection of the prescribed volume of air at the prescribed flow rate may be out of calibration at different environmental conditions. The pre-concentration step increases the time required for the measurement, sometimes to times longer than suitable for on-line use.

To improve the selectivity of species selective coatings for pre-concentrators, future polymer developments that enable an increasing percentage of multiple polymer interactions with each nitro functional group of the polynitroaromatics holds the promise of an increase in polymer-nitroaromatic air partition coefficients and hence sensor signals. In addition, as the polymer interaction with increasing numbers of target molecule functional groups increases, the selectivity of the polymer coated sensors relative to other background vapors will be substantially increased (Houser et al.).

DNT: <100 ppt (volume); interference from water vapor (Houser et al.)

Applicable References

27. Psillakis E, Kalogerakis N, 2001. Application of solvent microextraction to the analysis of nitroaromatic explosives in water samples. *J. Chromatog. A* 907: 211-219.
28. Houser EJ, Mlsna TE, Nguyen VK, Chung R, Mowery RL, McGill RA, 2001. *Talanta* 54: 469–485
29. Stahl DC, Tilotta DC, 2001. *Environ. Sci. Technol.* 35:3507-3512.
30. Furton KG, Almirall JR, Bi M, Wang J, Wu L. 2000. *J. Chromatography A* 885:419-432.
31. Wendel GJ, Bromberg EEA, Durfee MK. 1996. *Proc. Symp. Explosives Detection Technology, 2nd*, ed. WH Makky, pp. 181–86. Atlantic City: FAA
32. Settles GS, Gowadia HA, Strine SB, Johnson TE. 1996. *Proc. Symp. Explosives Detection Technology, 2nd*, ed. WH Makky, pp. 65–70. Atlantic City: FAA
33. Parmeter JE, Linker KL, Rhykerd CL Jr, Hannum DW. 1996. *Proc. Symp. Explosives Detection Technology, 2nd*, ed. WH Makky, pp. 187–92. Atlantic City: FAA
34. Mercado A, Marsden P. 1995. *Proc. Int. Workshop on Ion Mobility Spectrometry*, pp. 168–89. NASA Conf. Publ. 3301
35. Arnold JT. 1994. *SPIE Proc.* 2276:412–23
36. McGann W, Jenkins A, Ribeiro K. 1992. in *Proc. Int. Symp. Explosive Detection Technology, 1st*. Atlantic City: FAA pp. 518–531.
37. Fine DH, Achter EK. 1992. *Symposium on Access Security Screening: Challenges and Solutions, New Orleans, LA, ASTM Spec. Tech. Publ. 1127*, pp. 45–49. Philadelphia: ASTM
38. Davidson WR, Stott WR, Sleeman R, Akery AK. 1994. *SPIE Proc.* 2092:108–19
39. Achter EK, Miskolczy G, Fraim FW, Hainsworth E, Hobbs JR. 1992. in *Proc. Int. Symp. Explosive Detection Technology, 1st*. Atlantic City: FAA, pp. 427–434

40. Jankowski PZ, Mercado AG, Hallowell SF. 1993. *SPIE Proc.* 1824:13–24
41. Fine DH, Wendel GJ. 1994. *SPIE Proc.* 2092:131–36
42. Sheldon TG, Lacey RJ, Smith GM, Moore PJ, Head L. 1994. *SPIE Proc.* 2092:145–60
43. Ritchie RK, Thomson PC, DeBono RF, Danylewych-May LL, Kim L. 1994. *SPIE Proc.* 2092:87–93
44. Bennett G, Sleeman R, Davidson WR, Stott WR. 1994. *SPIE Proc.* 2276:363–71
45. Nacson S, Legrady O, Siu T, Greenberg D, Nargolwalla S, Geblewicz P. 1994. *SPIE Proc.* 2276:69–78
46. Fraim FW, Achter EK, Carroll AL, Hainsworth E. 1992. In: *Proc. Int. Symp. Explosive Detection Technology, 1st.* Atlantic City: FAA, pp. 559–70
47. Jenkins A, McGann W, Ribeiro K. 1992. in *Proc. Int. Symp. Explosive Detection Technology, 1st.* Atlantic City: FAA, pp. 532–551
48. Bromberg EEA, Carroll AL, Fraim FW, Lieb DP. 1992. In: *Proc. Int. Symp. Explosive Detection Technology, 1st.* Atlantic City: FAA, pp. 552–58
49. Hobbs JR, Conde EP. 1992. In *Proc. Int. Symp. Anal. Detect. Explos., 4th, London.* Dordrecht: Kluwer, pp. 437–53
50. Bender E, Hogan A, Leggett D, Miskolczy G, MacDonald S. 1992. *J. Forensic Sci.* 37:1673–78
51. Liu BYH, Yoo SH, Davies JP, Gresham G, Hallowell SF. 1994. *SPIE Proc.* 2276:45–55
52. Conrad, F. J. Explosives detection. The problem and prospects. *Nuclear Materials Management*, 1984, 13, 212–215.
53. Fraim, F. W., Achter, E. K., Carroll, A. L. and Hainsworth, E. Efficient collection of explosive vapors, particles and aerosols. *First International Symposium on Explosive Detection Technology*, Atlantic City, NJ, 1991, pp. 559–570.
54. Nacson, S. Adsorption phenomena in explosive detection. *Fifth International Symposium on Analysis and Detection of Explosives*, Washington, DC, 1995, paper no. 41.
55. Neudorfl, P., McCooeye, M. A. and Elias, L. Testing protocol for surface-sampling detectors. In: Yinon J. (ed.), *Advances in Analysis and Detection of Explosives*, Kluwer Academic Publishers, Dordrecht, 1993, pp. 373–384.
56. Davidson, W. R., Stott, W. R., Sleeman, R. and Akery, A. K. Synergy or dichotomy-vapor and particle sampling in the detection of contraband. *Conference on Substance Detection Systems*, Innsbruck, Austria, 1993. *SPIE Proceedings*, 1994, 2092, 108–119.

2.1.3 Chromatography

2.1.3.1 Gas Chromatography

Concept

Chromatographic methods are used to separate components in a sample. A sample is pushed through a column by a carrier gas (which constitutes the mobile phase). The various materials in the sample, by virtue of different interactions of each component with the stationary phase in the column, move through the column at different speeds, so that they emerge at different “retention times” and are separated. The separated materials are detected by a device that responds with an intensity that is proportional to the concentration of the component in the mixture. Many different kinds of detectors are used for explosive materials, such as electron capture detectors (ECD), chemiluminescence (or thermal energy analyzer) detectors specific to nitrogen containing species, and surface acoustic wave (SAW) detectors.

Demonstrated materials with associated detection limits and matrix effects

GC-TEA: sub-pm (pico-molar) detection of NG, EGDN, DNT, TNT, PETN, and RDX in a mixture (Rounbehler et al.)

GC/ECD: 1 mg kg⁻¹ for di- and trinitroaromatics, 10 mg kg⁻¹ for mono-nitroaromatics, 3 mg kg⁻¹ for RDX, 25 mg kg⁻¹ for HMX, and between 10 and 40 mg kg⁻¹ for nitrate esters (nitroglycerine [NG] and pentaerythritol tetranitrate [PETN]) (Walsh).

SAW: pg range detection of TNT and RDX (Staples, et al.)

Applicable References

57. Weiss T, Angerer J, 2002. Simultaneous determination of various aromatic amines and metabolites of aromatic nitro compounds in urine for low level exposure using gas chromatography-mass spectrometry. *J. Chromatog. B* 778: 179-192
58. Groom CA, Beaudet S, Halasz A, Paquet L, Hawari J, 2001. Detection of the cyclic nitramine explosives hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX) and octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazine (HMX) and their degradation products in soil environments. *J Chromatog. A* 909: 53-60
59. Gordin A, Amirav A, 2000. SnifProbe: new method and device for vapor and gas sampling. *J. Chromatog. A* 903: 155-172
60. Sigman ME, Ma CY 2001. Detection limits for GC/MS analysis of organic explosives. *J. Forensic Sciences* 46: 6-11.
61. Walsh ME, 2001. *Talanta* 54:427–438
62. Sigman ME, Ma CY 1999. In-injection port thermal desorption for explosives trace evidence analysis. *Anal. Chem.* 71:4119-24
63. Staples, E. J., Watson, G. W. A gas chromatograph incorporating an innovative new surface acoustic wave (SAW) detector. *Pittsburgh Conference on Analytical Chemistry and Applied Spectroscopy*, New Orleans, LA, 1998, paper no. 1583CP.
64. Ertl H, Breit U, Kaltschmidt H, Oberpriller H. 1994. *SPIE Proc.* 2276:58–68
65. Holland PM, Mustacich RV, Everson JF, Foreman W, Leone M, et al. 1994. *SPIE Proc.* 2276:79–86

66. Hobbs JR, Conde EP. 1992. See Ref. 12, pp. 153–64
67. Kolla P. 1994. *J. Chromatogr.* 674:309–18
68. Palmer DA, Achter EK, Lieb D. 1993. *SPIE Proc.* 1824:109–19
69. Fox S, Hooley T. 1994. *SPIE Proc.* 2093:195–203
70. Nacson, S., McNelles, L., Nargolwalla, S. and Greenberg, D. Method of detecting taggants in plastic explosives. Airport trials and solubility of explosives. *Second Explosives Detection Technology Symposium & Aviation Security Technology Conference*, Atlantic City, NJ, 1996, pp. 38-48.
71. Fine, D. H., Lieb, D. and Ruffe, F. Principle of operation of the thermal energy analyzer for the trace analysis of volatile and non-volatile N-nitroso compounds. *Journal of Chromatography*, 1975, 107, 351-357.
72. Lafleur, A. L. and Mills, K. M. Trace level determination of selected nitroaromatic compounds by gas chromatography with pyrolysis/chemiluminescent detection. *Analytical Chemistry*, 1981, 53, 1202-1205.
73. Goff, E. U., Yu, W. C. and Fine, D. H. Description of a nitro/nitroso specific detector for the analysis of explosives. *International Symposium on Analysis and Detection of Explosives*, Quantico, VA, 1983, pp. 159-168.
74. Rounbehler, D. P., MacDonald, S. J., Lieb, D. P. and Fine, D. H. Analysis of explosives using high speed gas chromatography with chemiluminescent detection. *First International Symposium on Explosive Detection Technology*, Atlantic City, NJ, 1991, pp. 703-713.
75. Wohltjen, H. and Dessy, R. Surface acoustic wave probe for chemical analysis. 1. Introduction and instrument description. *Analytical Chemistry*, 1979, 51, 1458-1464.
76. Wohltjen, H. and Dessy, R. Surface acoustic wave probes for chemical analysis. 2. Gas chromatography detector. *Analytical Chemistry*, 1979, 51, 1465-1470.
77. Watson, G., Horton, W. and Staples, E. Vapor detection using SAW sensors. *First International Symposium on Explosive Detection Technology*, Atlantic City, NJ, 1991, pp. 589-603.

2.1.3.2 HPLC

Concept

The direct chromatographic separation of liquid samples and detection of the components by a variety of means can be accomplished using high performance liquid chromatographic (HPLC) techniques. In fact, the EPA standard method for trace explosive residue detection in environmental samples is EPA Method 8330, which utilizes HPLC separation and UV detection. Dilute aqueous samples are pre-concentrated using a salting out procedure into acetonitrile, and then injected onto the HPLC column. Soil samples are extracted directly into acetonitrile. There have been a number of improvements and extensions of HPLC methods, mostly to reduce sample preparation and produce a method that is more real-time and field portable. These

improvements have mostly centered on improving the interface and utilizing SPME devices and improving the sample injection interface. Recently, the Swedes have developed a method to determine explosives in the vapor phase using on-line coupling of supercritical fluid extraction with high-performance liquid chromatography

Demonstrated materials with associated detection limits and matrix effects

EPA 8330 mix: <10 ng/mL each component (Wu et al.)

EPA mix: ca. 10-50 ng on porous graphite filter (after SFE) (Batlle et al.)

Applicable References

78. Wissinger CE, McCord BR, 2002. A gradient reversed phase HPLC procedure for smokeless powder comparison. J. Forens. Sci. 47: 168-174
79. Schreiber A, Efer J, Engewald W 2000. Application of spectral libraries for high-performance liquid chromatography-atmospheric pressure ionisation mass spectrometry to the analysis of pesticide and explosive residues in environmental samples. J. Chromatography A 869: 411-425
80. Batlle R, Carlsson H, Holmgren E, Colmsjo A, Crescenzi C, 2002. Journal of Chromatography A, 963:73-82
81. Lang MJ, Burns SE, 1999. Improvement of EPA method 8330: complete separation using a two-phase approach. J. Chromatog. A 849: 381-388
82. Wu L-M, Almirall JR, Furton KG 1999. J. High Resol. Chromatogr. 22, (5) 279-282
83. EPA Method 8330: www.epa.gov/epaoswer/hazwaste/test/pdfs/8330.pdf

2.1.3.3. Capillary electrophoresis

Concept

Separation of ionic species is achieved by the difference in mobility through a fluid driven by a potential difference. Detection is usually accomplished using a change in conductivity. McCord et al. demonstrated the separation and detection of components in a mixture of environmental decomposition products. Wang et al. have demonstrated a chip-based CE-conductivity microsystem for the rapid separation and detection of ions related to ammonium nitrate based explosives. The new microfluidic device offers significant advantages in term of speed, cost and sample size.

Demonstrated materials with associated detection limits and matrix effects

Separated 8 ions associated with ammonium nitrate based explosive post blast residues (Wang et al).

Applicable References:

84. Wang J, Pumera M, Collins G, Opekar, F, Jelinek I, 2002. Analyst, 2002, 127, 719-723

85. Thormann W, Lurie IS, McCord B, Marti U, Cenni B, Malik N, 2001. Advances of capillary electrophoresis in clinical and forensic analysis (1999-2000). *Electrophoresis* 22: 4216-4243

86. McCord BR, Hargadon KA, Hall KE, and Burmeister SG, 1994. *Anal. Chim. Acta*, **288**:43.

2.1.4 Mass spectrometry

Concept

A mass spectrometer separates materials according to the mass to charge ratio of the molecule and its fragments. A sample is introduced into a high vacuum chamber by various means, where it is ionized using a variety of methods, such as ion impact, electron impact, VUV, resonance enhanced multiphoton ionization (REMPI). The resultant ions are then accelerated into the spectrometer, which separates them based on geometric path (as in magnetic sector, quadrupole, or ion trap instruments) or time of flight. Conventional type instruments that have been used specifically to detect explosives are: an atmospheric pressure ionization (API) tandem mass spectrometer, an atmospheric sampling glow discharge ion trap mass spectrometer (ASGDI), and an API TOF mass spectrometer. Several instruments have been developed that take advantage of the large electron attachment cross sections of a large number of explosives. These include a reversal electron attachment mass spectrometer (READ) and an electron-capture negative ion mass spectrometer (ECNIMS). This latter instrument allows differentiation between various explosives containing NO_2^- fragment ions and between explosives and other nitrocompounds, by observing the electron energy at which the NO_2^- ion is formed. Materials containing C- NO_2 , O- NO_2 , and N- NO_2 bonds can be easily differentiated.

Demonstrated materials with associated detection limits and matrix effects

ASGDI	RDX: < pg (S.A. McLuckey, et al)
API-TOF-MS	TNT: 10 fg (H.G. Lee et al)
READ	TNT: < 100 pg (S. Boumsellek et al.)
ECNIMS	PETN: 20 pg detection limit (J.A. Laramie et al.)
CONDOR APCI MS/MS	RDX 0.59 pg, PETN 5.2 pg, TNT 0.39 pg (Stott et al.)
ITMS	TNT 0.01 pg (Asano et al.)

Applicable References

87. Hankin SM, Tasker AD, Robson L, Ledingham KWD, Fang X, McKenna P, McCanny T, Singhal RP, Kosmidis C, Tzallas P, 2002. Femtosecond laser time-of-flight mass spectrometry of labile molecular analytes: laser-desorbed nitro-aromatic molecules. *Rapid Comm. Mass Spec.* 16: 111-116
88. Wu ZG, Hendrickson CL, Rodgers RP, Marshall AG, 2002. Composition of explosives by electrospray ionization Fourier transform ion cyclotron resonance mass spectrometry. *Anal. Chem.* 74: 1879-1883
89. Evans CS, Sleeman R, Luke J, Keely BJ, 2002. A rapid and efficient mass spectrometric method for the analysis of explosives. *Rapid Comm. Mass Spec.* 16: 1883-1891

90. Costanza J, Davis WM, 2000. Rapid detection of volatile organic compounds in the subsurface by membrane introduction into a direct sampling ion-trap mass spectrometer. *Field Anal. Chem. Technol.* 4: 246-254.
91. Cassada DA, Monson SJ, Snow DD, Spalding RF, 1999. Sensitive determination of RDX, nitroso-RDX metabolites, and other munitions in ground water by solid-phase extraction and isotope dilution liquid chromatography-atmospheric pressure chemical ionization mass spectrometry. *J. Chromatog. A* 844: 87-95
92. McAvoy Y, Dost K, Jones DC, Cole MD, George MW, Davidson G 1999. A preliminary study of the analysis of explosives using packed-column supercritical fluid chromatography with atmospheric pressure chemical ionisation mass spectrometric detection. *Forensic Sci. Int.* 99: 123-141
93. McDowell, C. A. *Mass Spectrometry*, McGraw Hill, New York, 1963.
94. Dawson, P. H. Principles of operation. In: Dawson P. H. (ed.), Elsevier, Amsterdam, 1976, pp. 9-64.
95. Loans, J. N., Cooks, R. G., Syka, J. E. P., Kelley, P. E., Stafford, Jr., G. C. and Todd, J. F. J. Instrumentation, applications, and energy deposition in quadrupole ion-trap tandem mass spectrometry. *Analytical Chemistry*, 1987, 59, 1677-1685.
96. Cooks, R. G., Glush, O. L., McLuckey, S. A. and Kaiser, R. E. Ion trap mass spectrometry. *Chemical & Engineering News*, 1991, pp. 26-41.
97. McLafferty, F. W. Tandem mass spectrometry. *Science*, 1981, 214, 280-287.
98. Yinon, J. MS/MS techniques in forensic science. In: Maehly, A. and Williams, R. L. (eds), *Forensic Science Progress*, Vol 5, Springer-Verlag, Heidelberg, 1991, pp. 1-29.
99. Yost, R. A. and Enke, C. G. Triple quadrupole mass spectrometry for direct mixture analysis and structure elucidation. *Analytical Chemistry*, 1979, 51, 1251A-1264A.
100. Quarmby, S. T. and Yost, R. A. An improved method for performing a scan function on a quadrupole ion trap mass spectrometer. US Patent No. 08/837,030. April 15, 1997.
101. Yinon, J., McClellan, J. E. and Yost, R. A. Electrospray ionization tandem mass spectrometry collision-induced dissociation study of explosives in an ion trap mass spectrometer. *Rapid Communications in Mass Spectrometry*, 1997, 11, 1961-1970.
102. Davidson, W. R., Thomson, B. A., Akery, A. K. and Sleeman, R. Modifications to the ionization process to enhance the detection of explosives by API/MS/MS. First International Symposium on Explosive Detection Technology, Atlantic City, NJ, 1991, pp. 653-662.
103. Davidson, W. R., Stott, W. R., Akery, A. K. and Sleeman, R. The role of mass spectrometry in the detection of explosives. *First International Symposium on Explosive Detection Technology*, Atlantic City, NJ, 1991, pp. 663-671.
104. Sleeman, R., Bennett, G., Davidson, W. R. and Fisher, W. The detection of illicit drugs and explosives in real-time by tandem mass spectrometry. *International Symposium on Contraband and Cargo Inspection Technologies*, Washington, DC, 1992, pp. 57-63.

105. Stott, W. R., Davidson, W. R. and Sleeman, R. High throughput real time chemical contraband detection. *Conference on Substance Detection Systems*, Innsbruck, Austria, 1993. SPIE Proceedings, 1994, 2092, 53-63.
106. Bennett, G., Sleeman, R., Davidson, W. R. and Stott, W. R. An airport trial of a system for the mass screening of baggage or cargo. Conference on Cargo Inspection Technologies, San Diego, CA, 1994. *SPIE Proceedings*, 1994, 2276, 363-371.
107. McLuckey, S. A., Glish, G. L., Asano, K. G. and Grant, B. C. Atmospheric sampling glow discharge ionization source for the determination of trace organic compounds in ambient air. *Analytical Chemistry*, 1988, 60, 2220-2227.
108. McLuckey, S. A., Gush, G. L. and Asano, K. G. Coupling of an atmospheric sampling ion source with an ion-trap mass spectrometer. *Analytica Chimica Acta*, 1989, 225, 25-35.
109. Chutjian, A. and Darrach, M. R. Improved, portable reversal electron attachment (READ) vapor detection system for explosives detection. *Second Explosives Detection Technology Symposium & Aviation Security Technology Conference*, Atlantic City, NJ, 1996, pp. 176-180.
110. Yinon, J., Boettger, H. G. and Weber, W. P. Negative-ion mass spectrometry. A new analytical method for the detection of TNT. *Analytical Chemistry*, 1972, 44, 2235-2237.
111. Yinon, J. and Boettger, H. G. Modification of a high resolution mass spectrometer for negative ionization. *International Journal of Mass Spectrometry and Ion Physics*, 1972/73, 10, 161-168.
112. Laramee, J. A., Kocher, C. A. and Deinzer, M. L. Application of a trochoidal electron monochromator/mass spectrometer system to the study of environmental chemicals. *Analytical Chemistry*, 1992, 64, 2316-2322.
113. Laramee, J. A., Cody, R. B., Herrmannsfeldt, W. B. and Deinzer, M. L. Tunable energy electron monochromator interface to a sector instrument. *44th ASMS Conference on Mass Spectrometry and Allied Topics*, Portland, OR, 1996, p. 71.
114. Laramee, J. A. and Deinzer, M. L. Tunable energy (0.03-30 eV) electron capture negative ion mass spectrometry. *Fifth International Symposium on Analysis and Detection of Explosives*, Washington, DC, 1995, Paper No. 49.
115. Davidson WR, Stott WR, Akery AK, Sleeman R. 1992. In: *Proc. Int. Symp. Explosive Detection Technology, 1st*. Atlantic City: FAA, pp. 663-71
116. Yinon J. 1982. *Mass Spectrom. Rev.* 1:257-307
117. Burrows EP. 1992. In : *Proc. Int. Symp. Anal. Detect. Explos., 4th, London*. Dordrecht: Kluwer, pp. 299-307
118. Chen TH. 1992. In : *Proc. Int. Symp. Anal. Detect. Explos., 4th, London*. Dordrecht: Kluwer, pp. 385-401
119. Boumsellek S, Alajajian SH, Chutjian A. 1992. *J. Am. Soc. Mass Spectrom.* 3:243-47
120. Boumsellek S, Chutjian A. 1992. *Anal. Chem.* 64(18):2096-100
121. Chutjian A, Boumsellek S, Alajajian SH. 1992. In: *Proc. Int. Symp. Explosive Detection*

Technology, 1st. Atlantic City: FAA, pp. 571–83

122. Chutjian A, Darrach MR. 1996. In: *Proc. Explosives Detection Technology Symp. Aviation Security Technology Conf., 2nd*, Atlantic City: FAA, pp. 176–80
123. Davidson WR, Thomson BA, Sakuma T, Stott WR, Akery AK, Sleeman R. 1992. In: *Proc. Int. Symp. Explosive Detection Technology, 1st.* Atlantic City: FAA, pp. 653–62
124. Wright AD, Jennings KR, Peters R. 1992. In : *Proc. Int. Symp. Anal. Detect. Explos., 4th, London.* Dordrecht: Kluwer,, pp. 291–98
125. Xu Y, Herman JA. 1992. *Rapid Commun. Mass Spectrom.* 6(7):425–28
126. Giam CS, Ahmed MS, Weller RR, Derrickson J. 1992. In: *Proc. Int. Symp. Explosive Detection Technology, 1st.* Atlantic City: FAA, pp. 687–88
127. Giam CS, Holliday TL, Ahmed MS, Reed GE, Zhao G. 1994. *SPIE Proc.* 2092:227–37
128. Langford ML, Todd JFJ. 1993. *Org. Mass Spectrom.* 28:773–79
129. Crellin KC, Widmer M, Beauchamp JL. 1997. *Anal. Chem.* 69(6):1092–101
130. Stott WR, Green D, Mercado A. 1994. *SPIE Proc.* 2276:87–97
131. Cappiello A, Famiglini G, Lombardozzi A, Massari A, Vadalìa GG. 1996. *J. Am. Soc. Mass Spectrom.* 7(8):753–58
132. Zhao J, Zhu J, Lubman DM. 1992. *Anal. Chem.* 64(13):1426–33
133. Huang SD, Kolaitis L, Lubman DM. 1987. *Appl. Spectrosc.* 41(8):1371–76
134. Bryden WA, Benson RC, Ecelberger SA, Phillips TE, Cornish T, Cotter RJ. 1995. *SPIE Proc.* 2511:153–64
135. Glish GL, McLuckey SA, Grant BC, McKown HS. 1992. In: *Proc. Int. Symp. Explosive Detection Technology, 1st.* Atlantic City: FAA, pp. 642–52
136. Asano KG, Goeringer DE, McLuckey SA. 1995. *Anal. Chem.* 67(17):2739–42
137. McLuckey SA, Goeringer DE, Asano KG, Vaidyanathan G, Stephenson JL Jr. 1996. *Rapid Commun. Mass Spectrom.* 10(3):287–98
138. Lee HG, Lee ED, Lee ML. 1992. *Proc. Int. Symp. Explosive Detection Technol., 1st*, ed. SM Khan, pp. 619–33. Atlantic City: FAA

2.1.5 Ion mobility spectrometry

Concept

An ion mobility spectrometer consists of a sample inlet system, an atmospheric pressure ion source, an ion-molecule reactor, an ion-drift spectrometer, and a detector. Sample ions formed in the reactor are swept into the drift region by an applied electric field. They are separated according to their mobility as they travel through the drift gas; their mobility depends on their mass/charge ratio. Usually, mobilities are ratioed because the ratio is independent of operating conditions and permits use of internal standards for calibration. The long history of the use of

IMS to detect explosives coupled with strong understanding of the species produced in the ionization process for typical explosives make IMS widely utilized in the field. A newer variant known as transverse field compensation IMS (Carnahan et al.) eliminates the gating electrodes needed to pulse ions in conventional IMS so that ions are continuously injected. Instead two oscillating electric fields are applied in the drift region. Sweeping the second (compensating) field through a voltage range produces the spectrum.

Demonstrated materials with associated detection limits and matrix effects

Difficult to quantify. Usually used as an alarm for presence of a species, rather than for quantification. Suffers from masking by other species in the environment or false alarms by non-explosive species. Needs an additional orthogonal analytical method to reduce false alarm rate as well as to provide quantification. Hill and Simpson said "It is still difficult to find good quantitative data...for IMS)."

GC/IMS TNT: 5 pg (Simpson et al)

Applicable References

139. Eiceman GA, 2002. Ion-mobility spectrometry as a fast monitor of chemical composition. TRAC 21:259-275
140. Collins DC, Lee ML Developments in ion mobility spectrometry-mass spectrometry. 2002. Anal. Bioanal. Chem. 372:66-73
141. Li F, Xie Z, Schmidt H, Sielemann S, Baumbach JI. 2002. Ion mobility spectrometer for online monitoring of trace compounds. Spectrochim. Acta B 57: 1563-74.
142. Tabrizchi M, Abedi A, 2002. A novel electron source for negative ion mobility spectrometry. Int. J. Mass. Spec. 218: 75-85.
143. Asbury GR, Klasmeier J, Hill HH, 2000. Analysis of explosives using electrospray ionization/ion mobility spectrometry (ESI/IMS.) Talanta 50: 1291-1298
144. Ewing RG, Atkinson DA, Eiceman GA, Ewing GJ. 2001. Talanta 54:515-529.
145. Eiceman GA, Preston D, Tiano G, Rodriguez J. Parmeter JE, 1997. Talanta 45:57-74.
146. Hill HH, Simpson G. 1997. *Field Anal. Chem. Technol.* 1:119-34
147. Garafolo F, Migliozi V, Roio B. 1994. Rapid Commun. Mass Spec. 8:527-532.
148. Karpas, Z. Forensic science applications of ion mobility spectrometry. *Forensic Science Review*, 1989, 1, 103-119.
149. St. Louis, R. H. and Hill, Jr., H. H. Ion Mobility Spectrometry in Analytical Chemistry. *Critical Reviews in Analytical Chemistry*, 1990, 21, 321-355.

150. Fetterolf, D. D. and Clark, T. D. Detection of trace explosive evidence by ion mobility spectrometry. *Journal of Forensic Sciences*, 1993, 38, 28-39.
151. Danylewych-May, L. L. and Cumming, C. Explosive and taggant detection with lonscan. In: Yinon J. (ed.), *Advances in Analysis and Detection of Explosives*, Kluwer Academic Publishers, Dordrecht, 1993, pp. 385-401.
152. Anon, Examining the analytical capabilities of a new hand portable gas chromatography/ion mobility spectrometry system. <http://femtoscanner.com/analcap.htm>, Application Note No. 9702, FemtoScan Corporation, 1998.
153. Ritchie RK, Kuja F, Jackson RA, Loveless AJ, Danylewych-May LL. 1994. *SPIE Proc.* 2092:76–86
154. Fetterolf DD, Clark TD. 1992. In: *Proc. Int. Symp. Explosive Detection Technology, 1st*. Atlantic City: FAA, pp. 689–702
155. Fetterolf DD. 1992. In: *Proc. Int. Symp. Anal. Detect. Explos., 4th, London*. Dordrecht: Kluwer, pp. 117–31
156. Fetterolf DD, Donnelly B, Lasswell LD. 1994. *SPIE Proc.* 2092:40–52
157. Hallowell SF, Davies JP, Gresham BL. 1994. *SPIE Proc.* 2276:437–48
158. McGann WJ, Jenkins A, Ribiero K, Napoli J. 1994. *SPIE Proc.* 2092:64–75
159. McGann WJ, Bradley V, Borsody A, Lepine S. 1994. *SPIE Proc.* 2276:424–36
160. Lawrence AH, Goubran RA, Hafez HM. 1993. *SPIE Proc.* 1824:97–108
161. Danylewych-May LL. 1992. In: *Proc. Int. Symp. Explosive Detection Technology, 1st*. Atlantic City: FAA, pp. 672–86
162. Simpson G, Klasmeier M, Hill H, Atkinson D, Radolovich G, et al. 1996. *J. High Resol. Chromatogr.* 19:301–12
163. Carnahan BL, Day S, Kouznetsov V, Tarassov A. 1997. *SPIE Proc.* 2937: 106–19

2.1.5.1 Ion drift non-linearity spectrometry

Concept

Similar to IMS. May be terminology difference due to Russian authors.

Applicable references

164. Buryakov IA, Kolomiets YN, Luppou BV, 2001. *J. Anal. Chem*, 56: 336–340.
165. Buryakov, IA, Kolomiets YN, Louppou VB, 1999. *Proc. 8 Int. Conf. on IMS*, UK, Buxton

2.1.6 Infrared absorption spectroscopy

Concept

Molecular vibrations have characteristic frequencies in the infrared spectral range (a few cm^{-1} to several thousand cm^{-1}). Resonant absorption of light by these vibrations can be observed when light of the appropriate frequency is present, and when there is a change in the molecular dipole moment for that particular molecular vibration. Vibrations involving the NO_2 moiety have strong infrared absorption signatures, and their vibrational frequencies depend characteristically on the molecule, so that they can be used as a fingerprint. Infrared spectra of large molecules in the vapor phase can be quite complicated, as well as have large bandwidths, which leads to indistinct spectra. Also, in order to achieve high enough vapor pressures to allow detection, a large number of explosives decompose, so that the spectra are further complicated by the decomposition products (but see below for a use for this idea). Typical absorption cross sections (peak values, not band integrated) for NO_2 stretching modes in explosives are in the range $1\text{--}10 \times 10^5 \text{ cm}^2/\text{mol}$. Therefore a cell with 100 cm path length allows detection of 10 ppm (by volume) of vapor, which is pretty poor (TNT at 60°C).

Recently solid phase microextraction (SPME) methods have been coupled with IR absorption spectroscopy of the SPME films to determine nitroaromatics in water. The SPME polymer film has no absorption bands in the NO_2 stretch region to interfere with the analyte peaks.

Finally, selective absorption coatings on SAW devices have been coupled to FTIR via attenuated total reflection (ATR) methods. Selective coatings for DNT and TNT have recently been achieved via self assembly of cyclodextrin monolayers (Yang et al.).

Demonstrated materials with associated detection limits and matrix effects

IR vapor phase: 10 ppm TNT (Janni et al.)

SPME/IR: 50 $\mu\text{g/L}$ TNT (Stahl)

Applicable References

166. Yang XG, Du XX, Shi JX, Swanson BI, Talanta 54 (2001) 439–445
167. Stahl DC, Tilotta DC, 2001. Environ. Sci. Technol. 35:3507-3512.
168. Janni, J., Gilbert, B. D., Field, R. W. and Steinfeld, J. I. Infrared absorption of explosive molecule vapors. Spectrochimica Acta Part A, 1997, 53, 1375-1381.
169. Tung YS, Mu R, Henderson DO, Curby WA. 1997. *Appl. Spectrosc.* 51:171–77
170. Clapper M, Demirgian J, Robitaille G. 1996. *Spectroscopy* 10(7):44–49
171. Riris H, Carlisle CB, McMillen DF, Cooper DE. 1996. *Appl. Opt.* 35(24):4694–704
172. Wormhoudt J, Shorter JH, McManus JB, Kebabian PL, Zahniser MS, et al. 1996. *Appl. Opt.* 35:3992–97
173. Rohe T, Grunblatt E, Eisenreich N. 1996. *Proc. Int. Annu. Conf. Fraunhofer Inst. Chem. Technol.*, pp. 85-1–85-10
174. Henderson DO, Silberman E, Chen N, Snyder FW. 1993. *Appl. Spectrosc.* 47:528–32
175. Henderson DO, Mu R, Tung YS, Huston GC. 1995. *Appl. Spectrosc.* 49:444–50

176. Mercado A, Davies JP. 1994. *SPIE Proc.* 2092:27–37
177. Henderson, D. O., Silberman, E. and Snyder, F. W. Fourier-transform infrared spectroscopy applied to explosive vapor detection. First International Symposium on Explosive Detection Technology, Atlantic City, NJ, 1991, pp. 604–617.
178. Pristera F, Halik M, Castelli A, Fredericks W. 1960. *Anal. Chem.* 32:495–508
179. Chasan DE, Norwitz G. 1972. *Microchem. J.* 17:31–60
180. Iqbal Z, Suryanarayanan K, Bulusu S, Autera JR. 1972. *Infrared and Raman Spectra of 1,3,5-trinitro-1,3,5-triazacyclohexane (RDX)*, Rep. AD-752899, US Army Picatinny Arsenal, Dover, NJ
181. Eisenreich N, Kull H, Hertz J. 1994. *Proc. Int. Annu. Conf. Fraunhofer Inst. Chem. Technol.*, pp. 86-1–86-7
182. Cavagnat D, Lespade L, Lapouge C. 1995. *J. Chem. Phys.* 103:10502–12
183. Claspy PC, Pao Y-H, Kwong S, Novov E. 1977. *Appl. Opt.* 15:1506–9
184. Karpowicz RJ, Brill TB. 1984. *J. Phys. Chem.* 88:348–52
185. Carper WR, Stewart JJP. 1987. *Spectrochim. Acta* 43A:1249–55
186. Stelson AW, Friedlander SK, Seinfeld JH. 1979. *Atmos. Environ.* 13:369–72
187. Stelson AW, Seinfeld JH. 1982. *Atmos. Environ.* 16:983–92
188. Hong TZ, Tang CP, Lin K. 1992. In: *Proc. Int. Symp. Anal. Detect. Explos., 4th, London*. Dordrecht: Kluwer, pp. 145–52

2.1.6.1 IR detection of decomposition products

Concept

The predisposition of energetic materials to decompose on heating, lead a group of researchers to design a detector for the stable decomposition fragments and drive the decomposition process using a catalyst. The molecular fragments are then detected using frequency modulation spectroscopy with diode lasers. Thermal decomposition and detection of the fragments are also the means for operation of the Thermedics Detection EGIS system in use at many airports. The fragments have also been detected using Stark-modulated millimeter wave spectroscopy (Lovas et al.).

Fragmentation can also be induced via laser decomposition techniques. Coupling laser decomposition to multi-photon ionization methods can result in excellent detection limits (Lemire et al.).

Demonstrated materials with associated detection limits and matrix effects

RDX: 5-10 pg (H. Riris, et al.)

TNT: 3 pg; RDX: 1 pg (Lemire et al.)

Applicable References

189. Wormhoudt J, Kebabian PL, Kolb CE. 1997. *Combust. Flame* 111:73–86
190. Riris, H., Carlisle, C. B., McMillen, D. F. and Cooper, D. E. Explosives detection with a frequency modulation spectrometer. *Applied Optics*, 1996, 35, 4694-4704.
191. Nelson DD, Zahniser MS, McManus JB, Shorter JH, Wormhoudt JC, Kolb CE. 1996. *SPIE Proc.* 2834:148–59
192. Wormhoudt J, Zahniser MS, Nelson DD, McManus JB, Miake-Lye RC, Kolb CE. 1995. *SPIE Proc.* 2546:552–61
193. Lovas FJ, Suenram RD. 1995. *Thermal Decomposition Pathways in Nitramine Propellants. Final Rep., USARO Contract 29596-CH*. Gaithersburg, MD: NIST
194. Zahniser MS, Nelson DD, McManus JB, Kebabian PL. 1995. *Philos. Trans. R. Soc. London Ser. A* 351:371–82
195. Hnatnický S. 1994. *J. Testing Eval.* 22(3):282–85
196. Fine DH, Rounbehler DP, Curby WA. 1992. In: *Proc. Int. Symp. Explosive Detection Technology, 1st*. Atlantic City: FAA, pp. 505–17
197. Lemire GW, Simeonsson JB, Sausa RC. 1993. *Anal. Chem.* 65:529–33

2.1.6.2 Cavity ring down spectroscopy*Concept*

The principle of CRDS is as follows. Light from a pulsed or CW laser source is injected into a stable optical cavity formed by two, or more, highly reflective mirrors. At the end of the laser pulse (or in the case of a CW laser, the laser is turned off) the intracavity radiation will decay exponentially with a time constant that is determined by the reflectivity of the mirrors the scattering inside the cavity (such as Rayleigh scattering of the gas sample), and the wavelength dependent absorption of the intracavity gas. Measurement of the ringdown time versus wavelength of the injection laser produces the equivalent of an absorption spectrum. A typical noise floor of a good cavity ringdown instrument in the mid-infrared (Todd et al.) is ca. $A = 1 \times 10^{-8}$. With typical NO_2 stretch band peak absorption cross sections of ca. $10^6 \text{ cm}^2/\text{mol}$ implies TNT would be detectable in the vapor at room temperature, but other materials would need some kind of pre-concentrator.

CRDS has also been done in using UV transitions of TNT in the vapor phase. The spectral selectivity for differentiation from other species is poor.

Demonstrated materials with associated detection limits and matrix effects

TNT: 1 ppb (volume) using UV transitions (Usachev et al.). Strong interference probabilities.

Applicable References

198. Todd MW, Provencal RA, Owano TG, Paldus BA, Kachanov A, Vodopyanov KL, Hunter M, Coy SL, Steinfeld JJ, Arnold JT, 2002. *Appl. Phys. B* 75:367-76

199. Usachev AD, Miller TS, Singh JP, Yueh FY, Jang PR, Monts DL, 2001. Appl. Spectrosc., 55: 125-129

2.1.7 Optoacoustic spectroscopy

Concept

Optical energy absorbed by molecules is partially turned into thermal energy via non-radiative relaxation processes. The thermal energy can be detected via the rise in temperature and pressure in a cell containing the molecules of interest. If pulsed or chopped radiation is used for excitation, the pressure pulses can be detected using a sensitive microphone or piezoelectric transducer located within the cell. A photoacoustic absorption spectrum can be obtained by phase sensitively recording the normalized transducer signal versus wavelength of the excitation source. Often infrared laser sources are used and vibrational spectra are obtained, for the reasons discussed under infrared absorption (narrow transitions, large absorption cross sections, and species specific spectral features).

Demonstrated materials with associated detection limits and matrix effects

NG: 0.28 ppb; EGDN: 8.3 ppb; DNT: 0.5 ppb, but ambient levels of CO₂, H₂O, NH₃, and O₃ interfere strongly at the 9.6 μ m excitation wavelength (Crane).

Applicable References

200. Fulghum SF. 1993. *Detection of Explosives Vapor at the PPT Level with a Laser Interferometric Calorimeter*, Rep. SRL-05-F-1993, Sci. Res. Lab., Inc., Somerville, MA
201. Fulghum SF, Tilleman MM. 1991. *J. Opt. Soc. Am. B* 8:2401–13
202. Rosengren, L.-G. Optimal optoacoustic detector design. *Applied Optics*, 1975, 14, 1960-1976.
203. Claspy, P. C., Pao, Y.-H., Kwong, S. and Nodov, E. Laser optoacoustic detection of explosive vapors. *Applied Optics*, 1976, 15, 1506-1509.
204. Claspy, P. C. Infrared optoacoustic spectroscopy and detection. In: Pao Y.-H. (ed.), *Optoacoustic Spectroscopy and Detection*, Academic Press, New York, 1977, pp. 133-166.
205. Crane, R. A. Laser optoacoustic absorption spectra for various explosive vapors. *Applied Optics*, 1978, 17, 2097-2102.

2.1.8 UV/visible methods

Concept

UV/visible absorption spectra of typical explosives are broad and featureless, making their use for quantitative analysis difficult or impossible. However, the absorptions can provide resonance enhancement for other methods, such as Raman (UVRRS – see Mercado et al.). There are very

weak absorptions in the visible that are accessible via photoacoustic methods, but their weakness makes them not useable for detection at low concentrations.

Fluorescence or luminescence can be used for detection. Fluorescence from the species of interest can be discriminated from background fluorescence using multispectral imaging. Chemi- and bioluminescence have been used for selective detection of explosives (see Boncyk). The discrimination capabilities of enzyme reactions has been utilized in a bioluminescent sensor for TNT and RDX (VanBergen et al). See section 2.3.3 Immunochemical sensors.

Visible luminescence has been observed from thermally decomposed nitro-organic vapors in a tube furnace (Crowson et al).

Demonstrated materials with associated detection limits and matrix effects

TNT and RDX: 5 $\mu\text{g/L}$ (competitive fluorescence immunoassay – VanBergen et al.)

Applicable References

206. VanBergen SK, Bakaltcheva IB, Lundgren JS, Shriver-Lake LC, 2000. *Environ. Sci. Technol.* 34:704-708
207. Crowson A, Hiley RW, Ingham T, Mc-Creedy T, Pilgrim AJ, Townshend A. 1997. *Anal. Commun.* 34:213–16
208. Crowson A, Hiley RW, Ingham T, Mc- Creedy T, Pilgrim AJ, Townshend A. 1997. *Anal. Commun.* 34:213–16
209. Funsten HO, McComas DJ. 1997. *US Patent No. 5638166*
210. Wu DD, Singh JP, Yueh FY, Monts DL. 1996. *Appl. Opt.* 35(21):3998–4003
211. Mercado A, Janni J, Gilbert B, Steinfeld JI. 1996. In: *Proc. Explosives Detection Technology Symp. Aviation Security Technology Conf., 2nd*, Atlantic City: FAA,, pp. 91–99
212. Hasue K, Nakahara S, Morimoto J, Yamagami T, Okamoto Y, Miyakawa T. 1995. *Propellants Explos. Pyrotech.* 20(4):187–91
213. Zuckermann H, Greenblatt GD, Haas Y. 1987. *J. Phys. Chem.* 91:5159–61
214. Seitz, W. R. and Neary, M. P. Chemiluminescence and bioluminescence in chemical analysis. *Analytical Chemistry*, 1974, 46, 188A-202A.
215. Boncyk, E. M. A bioluminescent explosives vapor detection and identification system. Third International Symposium on Analysis and Detection of Explosives, Mannheim-Neuostheim, Germany, 1989, pp. 40.41-40.14.

2.1.9 Portals

Concept

Because invasive interrogation methods such as X-rays or nuclear methods cannot necessarily be used to screen people, a variety of other less invasive methods have been incorporated into portal

devices. The most commonly encountered portal is the ubiquitous walk through metal detector. Recent efforts have been aimed at increasing the efficiency of metal detection portals and incorporating other detection capabilities for explosives or other illicit substances. Technologies fall into two basic categories: imaging and trace detection. Advanced imaging systems include raster scan backscattered X-ray tomography, millimeter wave holography, microwave detection of dielectric function anomalies. Trace detection methods have required incorporating a variety of sampling paradigms to portals to enable collection of vapors and/or particles from subjects. These have included puffers or air jets, paddles, acoustic energy, and other types of airflow. The collected material is then analyzed using IMS, MS/ECD, and chemiluminescence methods, among others.

Applicable References

216. Hallowell SF. 2001. *Talanta* 54:447-458.
217. Rhykerd, C., Linker, K., Hannum, D. and Parmeter, J. Walk-through explosives detection portal. *Nuclear Materials Management*, 1997, 26, 97-102.
218. Wendel, G. J., Bromberg, E. E. A., Durfee, M. K. and Curby, W. Design of a walk-through trace EDS. *Second Explosives Detection Technology Symposium & Aviation Security Technology Conference*, Atlantic City, NJ, 1996, pp. 181-186.
219. Parmeter, J. E., Linker, K. L., Rhykerd, Jr., C. L. and Hannum, D. W. Testing of a walk-through portal for the trace detection of contraband explosives. *Second Explosives Detection Technology Symposium & Aviation Security Technology Conference*, Atlantic City, NJ, 1996, pp. 187-192.
220. Hobbs, J. R. and Conde, E. P. Analysis of airflows in personnel screening booths. In: Yinon J. (ed.), *Advances in Analysis and Detection of Explosives*, Kluwer Academic Publishers, Dordrecht, 1993, pp. 437-453
221. Bromberg, E. E. A., Dussault, D., MacDonald, S. and Curby, W. A. Vapor generation for use in explosive portal detection devices. In: Yinon J. (ed.), *Advances in Analysis and Detection of Explosives*, Kluwer Academic Publishers, Dordrecht, 1993, pp. 473-484.
222. Hintze, M. M., Hansen, B. L. and Heath, R. L. Real-time explosives/narcotics vapor enhancement and collection systems for use with the atmospheric pressure ionization time-of-flight mass spectrometer. *First International Symposium on Explosive Detection Technology*, Atlantic City, NJ, 1991, pp. 634-636.
223. Jenkins, A., McGann, W. and Ribeiro, K. Extraction, transportation and processing of explosives vapor in detection systems. *First International Symposium on Explosive Detection Technology*, Atlantic City, NJ, 1991, pp. 532-551.

2.1.10 Vapor and solid generators

Concept

In order to calibrate the various detection methods, means to generate known concentrations of explosive vapors and well-known solid particles are necessary. This has been accomplished in

various manners, including continuous thermal sources, transient methods using GC columns and injectors, and pulsed methods, usually using a pre-concentrator or precise mass of EM in a known volume.

Applicable References

Vapor Generators:

224. Eiceman, G. A., Preston, D., Tiano, G., Rodriguez, J. and Parmeter, J. E. Quantitative calibration of vapor levels of TNT, RDX, and PETN using a diffusion generator with gravimetry and ion mobility spectrometry. *Talanta*, 1997, 45, 57-74.
225. Hartell, M. G., Myers, L. J., Wagonner, P., Kuhiman, M., Hallowell, S. F. and Petrousky, J. A. Design and testing of a quantitative vapor delivery system. Fifth International Symposium on Analysis and Detection of Explosives, Washington, DC, 1995, Paper No. 48.
226. Hartell, M. G., Pierce, M. Q., Myers, L. J., Hallowell, S. F. and Petrousky, J. A. Comparative analysis of smokeless powder vapor signatures derived under static versus dynamic conditions. Fifth International Symposium on Analysis and Detection of Explosives, Washington, DC, 1995, Paper No. 46.
227. Stott, W. R., Green, D. and Mercado, A. Mass spectrometric detection of solid and vapor explosive materials. Conference on Cargo Inspection Technologies, San Diego, CA, 1994. SPIE Proceedings, 1994, 2276, 87-97.
228. Lucero, D. P., Roder, S. R., Jankowski, P. and Mercado, A. Design concept: Femtogram level explosives vapor generator. In: Yinon J. (ed.), *Advances in Analysis and Detection of Explosives*, Kluwer Academic Publishers, Dordrecht, 1993, pp. 485-502.
229. Davies, J. P., Blackwood, L. G., Davis, S. G., Goodrich, L. D. and Larsen, R. A. Design and calibration of pulsed vapor generators for TNT, RDX and PETN. In: Yinon J. (ed.), *Advances in Analysis and Detection of Explosives*, Kluwer Academic Publishers, Dordrecht, 1993, pp. 513-532.
230. Davies, J. P., Blackwood, L. G., Davis, S. G., Goodrich, L. D. and Larson, R. A. Design and calibration of pulsed vapor generators for 2,4,6-trinitrotoluene, cyclo- 1,3,5-trimethylene-2,4,6-trinitraflfline, and pentaerythritol tetranitrate. *Analytical Chemistry*, 1993, 65, 3004-3009.
231. Bromberg EEA, Dussault D, MacDonald S, CurbyWA. 1992. In : *Proc. Int. Symp. Anal. Detect. Explos., 4th, London*. Dordrecht: Kluwer., pp. 473-84
232. Kenna BT, Conrad FJ, Hannum DW. 1992. In: *Proc. Int. Symp. Explosive Detection Technology, 1st*. Atlantic City: FAA, pp. 510-17
233. Macdonald SJ, Rounbehler DP. 1992. In: *Proc. Int. Symp. Explosive Detection Technology, 1st*. Atlantic City: FAA, pp. 584-88
234. Reiner, G. A., Heisy, C. L. and McNair, H. M. A transient explosive vapor generator based on capillary gas chromatography. *Journal of Energetic Materials*, 1991, 9, 173-190.

Solid particle generators:

235. Davies JP, Hallowell SF, Hoglund DE. 1994. *SPIE Proc.* 2092:137–44
236. Elias L. 1994. *J. Test. Eval.* 22(3):280–81
237. Neudorfl P, McCooeye MA, Elias L. 1992. In : *Proc. Int. Symp. Anal. Detect. Explos., 4th, London.* Dordrecht: Kluwer,, pp. 373–84
238. Gresham GL, Davies JP, Goodrich LD, Blackwood LG, Liu BYH, et al. 1994. *SPIE Proc.* 2276:34–44

2.1.11 Surface Enhanced Raman Scattering

Concept

Metal nanostructures or nanoparticles can cause large enhancements (up to $\times 10^6$) of the Raman scattering cross section for molecules adsorbed on them. The origins of this effect have been in dispute, but recent advances in production of nanostructures with very precise control of their size, shape, and spacing have allowed both greater understanding of the origin of the effect and its control. Small metal nanoparticles or nanostructures have a localized surface plasmon resonance that appears to provide most of the Raman enhancement, maximized when the LSPR frequency overlaps that of the excitation laser. There also appears to be a small “chemical” contribution to the enhancement caused by changes in bond polarizability in an adsorbed molecule.

Early SERS experiments were not very reproducible due to variations in the roughness or surfaces that were first used, or to variable production of colloids or other small particles. Recently several different schemes have been developed to produce highly uniform and reproducible LSPR nanostructures from several different materials. Silver nanostructures are most common and provide to date the largest enhancements, but suffer from oxidation and other chemical attack. Gold nanostructures have the advantage of a large enhancement and chemical robustness. The production schemes include vapor deposition through self assembled monolayer masks, electrochemical etching protocols, templated self assembly of colloidal crystals, and annealing of vapor plated metal islands.

Such nanostructures have been used to detect TNT and DNT impurity in the vapor phase. They have also been used to detect selectively functionalized TNT with an additional enhancement due to the resonance Raman effect, with further improvement in detection limit.

Demonstrated materials with associated detection limits and matrix effects

PCA of SERS on OH treated electrochemically etched silver: < 5 ppb (Sylvia et al)

SERRS of functionalized TNT: < 1 nM

SERS of TNT on colloidal Au nanoparticles: < 1 pg (< 100 pM) (Kneipp et al. 1995)

Applicable References

239. McHugh CJ, Keir R, Graham D, Smith WE, 2002. *Chem. Commun.* 2002:580-81.
240. Jensen TR, Malinsky MD, Haynes CL, Van Duyne RP. 2000. *J. Phys. Chem. B* 104:10549-56
241. Tessier PM, Velez OD, Kalambur AT, Rabolt JF, Lenhof AM, Kaler EW, 2000. *J. Am. Chem. Soc.*

122:9554-5

- 242. Sylvia JM, Janni JA, Klein JD, Spencer KM, 2000. *Anal. Chem.* 72: 5831-40
- 243. Stöckle RM, Deckert V, Fokas C., Zenobi R, 2000. *Appl. Spectrosc.* 54:1577-83.
- 244. Kneipp K, Wang Y, Dasari RR, Feld MS, Gilbert BD, Janni J, Steinfeld JJ. 1995. *Spectrochim Acta A* 51:2171-75.
- 245. Freeman RG, Grabar KC, Allison KJ, Bright RM, Davis JA, et al. 1995. *Science* 267:1629–32
- 246. Grabar KC, Freeman RG, Hommer MB, Natan MJ. 1995. *Anal. Chem.* 67:735–43
- 247. Fleischmann M, Hendra PJ, McQuillan AJ. 1974. *Chem. Phys. Lett.* 26:163–65
- 248. Campion A. 1985. *Annu. Rev. Phys. Chem.* 36:549–72

2.2 Bulk detection

Concept

Rather than rely on being able to detect explosive vapors or aerosol particles, methods have been developed to observe the bulk materials in situ. As the bulk materials are likely to be containerized and hidden, effective methods are limited to penetrating electromagnetic radiation, low-energy radiowaves and microwaves, high energy X-rays and γ rays, and neutrons.

2.2.1 Electromagnetic radiation

2.2.1.1 X-rays

Concept

X-rays can be used in a number of ways to detect explosives. The common airport X-ray scanner uses W K α radiation (near 60 keV) imaging to provide excellent gray scale dynamic range to allow identification of metal objects but also lighter objects. The attenuated signal is supposed to be a measure of potential threat, but results in false alarms in nearly every case. So dual energy S-ray systems were developed, which make use of the fact that the photoelectric effect is strong dependent on Z number. Comparing images made at two different energies produces information about the effective Z of the examined object, but only approximately. The lower the X-ray energy, the better the discrimination, but the higher the absorption, so that a realistic lower limit for luggage is ca. 50 keV. The incident X-rays are also back scattered by the Compton effect, and the scattered photons can be used together with the absorption measurement to separate the effects of density and Z. One signature of explosives is high density and low Z. X-rays are also scattered in the forward direction. These can be detected at a slight angle and compared to the transmitted beam intensity. All three intensities (back scatter, forward scatter, transmission) have been used to locate sheet explosives in luggage.

Incident X-rays are also scattered at low angles. Energy analysis of scattered photons at a well defined angle provides information on the molecular structure of the scattering medium,

particularly because of diffraction effects in crystalline materials. The two most important parameters for selecting the best geometry are the need for good energy resolution (i.e., at high scattering angle) and high photon energy (for good transmission, i.e., at low scattering angle). The usual experimental compromise is a scattering angle of 4-5°. Most benign materials produce broad featureless energy spectra, but usual explosives exhibit characteristic diffraction peaks. A variant that has some advantages is angular dispersive X-ray diffraction. Tomographic energy-dispersive X-ray diffraction (EXDT) has been applied to detection of explosives in luggage, where 200 g pieces of explosive down to 5 mm thickness were found. Computed tomography has been used to image luggage. Scanning at two different source energies can map the spatial elements (voxels) according to effective Z and density. Objects hidden in one image behind an object of large X-ray absorptivity can be located using dual view and dual energy systems.

Applicable References

249. Grodzins, L. Photons in - photons out: Non-destructive inspection of containers using X-ray and gamma ray techniques. First International Symposium on Explosive Detection Technology, Atlantic City, NJ, 1991, pp. 201-231.
250. Grodzins, L. Nuclear techniques for finding chemical explosives in airport luggage. Nuclear Instruments and Methods in Physics Research B, 1991, 56/57, 829-833.
251. Anon. Technology against terrorism: The federal effort. US Congress, Office of Technology Assessment, Report No. OTA-ISC-48 1, Washington, DC, 1991.
252. Anon. Technology against terrorism: Structuring security. US Congress, Office of Technology Assessment, Report No. OTA-ISC-5 11, Washington, DC, 1992.
253. Condon, E. U. X-rays. In: Condon E. U. and Odishaw E. U. (eds.), Handbook of Physics, McGraw-Hill, New York, 1967, pp. 7.126-127.138.
254. Schafer, D., Annis, M. and Hacker, M. New X-ray technology for the detection of explosives. First International Symposium on Explosive Detection Technology, Atlantic City, NJ, 1991, pp. 269-281.
255. Aitkenhead, W. F. and Stilison, J. H. Dual energy X-ray Compton scattering measurement as a method to detect sheet explosives. Second Explosives Detection Technology Symposium & Aviation Security Technology Conference, Atlantic City, NJ, 1996, pp. 236-241.
256. Luggar, R. D., Horrocks, J. A., Speller, R. D. and Lacey, R. J. Low angle X-ray scatter for explosives detection: a geometry optimization. Applied Radiation and Isotopes, 1997, 48, 215-224.
257. Carter, T., Dermody, G., Pleasants, I. B., Burrows, D., Mackenzie, S. J., Jupp, I. D. and Ramsden, D. Angular resolved X-ray diffraction measurements of explosives. Sixth International Symposium on Analysis and Detection of Explosives, Prague, Czech Republic, 1998.
258. Hnatnicky, S. CXRS explosives detection airport prototype. Conference on Physics-based Technologies for The Detection of Contraband, Boston, MA, 1996. SPIE Proc. 1997, 2936, 180-190.

259. Harding, G., Newton, M. and Kosanetzky, J. Energy-dispersive X-ray diffraction tomography. *Physics in Medicine and Biology*, 1990, 35, 33-41.
260. Curry, I. T. S., Dowdey, J. E. and Murry, Jr., R. C. Christensen's *Physics of Diagnostic Radiology*, 4th ed., Lea & Febiger, Philadelphia, PA, 1990, p. 522.
261. Anon. Product overview. <http://www.invision-tech.com/products/prodover.htm>: In Vision Technologies, Newark, CA, 1998.
262. Dolan, K. W., Ryon, R. W., Schneberk, D. J., Martz, H. E. and Rikard, R. D. Explosives detection limitations using dual-energy radiography and computed tomography. *First International Symposium on Explosive Detection Technology*, Atlantic City, NJ, 1991, pp. 252-260.
263. Lu, Q. and Connors, R. W. X-ray image analysis for luggage detection. *Second Explosives Detection Technology Symposium & Aviation Security Technology Conference*, Atlantic City, NJ, 1996, pp. 242-247.
264. Willard, H. H., Merritt, Jr., L. L. and Dean, J. A. *Instrumental Methods of Analysis*, Van Nostrand Co., Princeton, NJ, 1961, p. 626.
265. Clifford, J. R., Miller, R. B., McCullough, W. F. and Habiger, K. W. An explosive detection system for screening luggage with high energy X-rays. *First International Symposium on Explosive Detection Technology*, Atlantic City, NJ, 1991, pp. 237-251.

2.2.1.2 Gamma rays

Concept

γ-rays lose energy on passage through matter in three ways: photoelectric effect, Compton effect, and pair production. An explosives detector has been developed using pair production by γ-rays. The γ-rays are produced by RF LINAC e-beam impinging on a W or Ta target, absorbed by nitrogen atoms in the sample, which decays producing a positron. Positron annihilation produces characteristic 511 keV photons that are coincidence detected. The system has good spatial resolution because the 511 keV annihilation photons are counted coincidentally. The explosive lies on the line between the two detectors at the crossing point of the γ-ray. Discrimination against other N containing species in the object depends on proper adjustment of the electron beam energy to allow selective activation of the N in the explosive. That depends on the photoneutron threshold of the N atom, which depends on its chemical bonding.

γ-ray nuclear resonance absorption has also been used to detect regions of high nitrogen content. ^{14}N has a nuclear transition at 9.17 MeV with minimal temperature broadening. This excited state can be reached by absorption of 1.75 MeV protons by ^{13}C . The de-excitation γ-rays are emitted in an axially symmetric cone at 80.7° from the proton beam direction. The emitted γ-rays then pass through the item to be inspected, and the attenuation is a measure of the projected nitrogen contents. They are then detected using a resonant absorption in a nitrogen rich medium followed by pulse shape discrimination of the scintillation light (which allows differentiation of the 1.5 MeV proton from the numerous Compton electrons produced in the detector by photons of all

energies). A variant of this method has been developed to detect compounds with large chlorine contents, such as ammonium perchlorate.

Applicable References

- 266. Sredniawski, J. J. Detecting concealed explosives with gamma rays. *The Industrial Physicist*, 1997, 3, 24-27.
- 267. Vartsky, D., Engler, G. and Goldberg, M. B. A method for detection of explosives based on nuclear resonance absorption of gamma rays in ^{14}N . *Nuclear Instruments and Methods in Physics Research A*, 1994, 348, 688-691.

2.2.1.3 NMR

Concept

Nuclear magnetic resonance spectroscopy is based on the absorption of RF energy by spinning nuclei in a strong magnetic field when the nuclei undergo transitions from one alignment in the applied field to an opposite one. Spectra are obtained either by varying the magnetic field strength at fixed RF frequency, or by varying the RF frequency at fixed magnetic field. The absorption frequency for each kind of nucleus depends on the electronic distribution around it, so that the frequency depends on the location of the nucleus in a molecular structure. Coupling of nuclei results in splitting of the resonance.

Pulsed hydrogen NMR has been used to detect explosives in parcels, letters, and luggage. The transient NMR method uses multiple transmitted RF pulses to determine the spin-lattice relaxation time T_1 , the free-induction decay time T_2 , and the ^1H - ^{14}N cross-coupling coefficient. Most common explosives have long T_1 and short T_2 that is distinguishable from other common solids and liquids, and characteristic ^1H - ^{14}N coefficients.

Applicable References

- 269. Rabenstein, D. L. Nuclear magnetic resonance spectroscopy. In: Gouw T. H. (ed.), *Guide to Modern Methods of Instrumental Analysis*, Wiley-Interscience, New York, 1972, pp. 231-278.
- 270. Hore, P. J. *Nuclear Magnetic Resonance*, Oxford University Press, Oxford, 1995.
- 271. McKay, D. R., Moeller, C. R., Magnuson, E. E. and Burnett, L. J. Liquid explosives screening system. *First International Symposium on Explosive Detection Technology*, Atlantic City, NJ, 1991, pp. 454-464.
- 272. Jelinski, L. W. Modern NMR spectroscopy. *Chemical & Engineering News*, 5 November 1984, 26-47.
- 273. King, J. D., De Los Santos, A., Nicholls, C. I. and Rollwitz, W. L. Application of magnetic resonance to explosives detection. *First International Symposium on Explosive Detection Technology*, Atlantic City, NJ, 1991, pp. 478-485.

274. King, J. D. Explosives detection-The case for magnetic resonance. In: Yinon J. (ed.), *Advances in Analysis and Detection of Explosives*, Kluwer Academic Publishers, Dordrecht, 1993, pp. 351-359.

2.2.1.4 ESR

Concept

ESR is based on the absorption of microwave energy when spinning electrons aligned in an external field flip between orientations in the field. Usually the field is a magnetic field, so that the energy states of the Zeeman states. In practice, the microwave energy is held fixed and the magnetic field strength is varied to produce the ESR spectrum. The magnetic behavior of a given electron in a molecule is altered by the local magnetic fields of the surrounding atoms, so that the absorption frequencies are molecule specific. ESR is limited to materials that contain free spins. ESR has been found to give exceptionally strong signals in black powder.

Demonstrated materials with associated detection limits and matrix effects

Black powder: < 1 mg (Poindexter et al.)

Applicable References

275. Poole, Jr., C. P. Electron spin resonance. In: Gouw T. H. (ed.), *Guide to Modern Methods of Instrumental Analysis*, Wiley-Interscience, New York, 1972, pp. 279-321.
276. Poindexter, E. H., Leupold, H. A., Wittstruck, R. H. and Gerardi, G. J. Consideration of untried magnetic resonance techniques for possible baggage analysis. *First International Symposium on Explosive Detection Technology*, Atlantic City, NJ, 1991, pp. 493-504.

2.2.1.5 NQR

Concept

NQR is similar to NMR, except the splitting between the energy states is due to the interaction of the nuclear quadrupole moment with a molecular gradient in the absence of any external perturbation. Therefore, NQR measurements have to be made in the solid phase at low temperature. The ^{14}N NQR absorption frequencies from RDX have been found to be quite unique. However, as NQR signals are quite weak and the limit on pulse repetition frequency is determined by T_1 to ca. 10 Hz, a more efficient alternative is to use steady state free precession (SSFP), wherein a steady stream of RF pulses produces a steady state signal. The signal to noise ratio advantage of SSFP for a given scan time is given by $1/2 (T_1/T_2)$. A prototype fieldable NQR system has detected RDX and PETN in luggage with high selectivity over other materials.

Applicable References

277. Laszlo, P. and Stang, P. J. *Organic Spectroscopy. Principles and Applications*, Harper & Row Publishers, New York, 1971.

278. Sanders, J. K. M. and Hunter, B. K. Modern NMR Spectroscopy. A Guide for Chemists, Oxford University Press, Oxford, 1988.
279. Garroway, A. N., Buess, M. L., Miller, J. B., McGrath, K. J., Yesinowski, J. P., Suits, B. H. and Miller, G. R. Nuclear Quadrupole resonance (NQR) for detection of explosives and landmines. Sixth International Symposium on Analysis and Detection of Explosives, Prague, Czech Republic, 1998.
280. Buess, M. L., Garroway, A. N., Miller, J. B. and Yesinowski, J. P. Explosives detection by ^{14}N pure NQR. In: Yinon J. (ed.), Advances in Analysis and Detection of Explosives, Kluwer Academic Publishers, Dordrecht, 1993, pp. 361-368.
281. Garroway, A. N., Buess, M. L., Yesinowski, J. P. and Miller, J. B. Narcotics and explosives detection by ^{14}N pure NQR. Conference on Substance Detection Systems, Innsbruck, Austria, 1993. SPIE Proceedings, 1994, 2092, 318-327.
282. Buess, M. L., Garroway, A. N. and Miller, J. B. NQR detection using a meanderline surface coil, Journal of Magnetic Resonance, 1991, 92, 348-362.
283. Rayner, T., Thorson, B., Beevor, S., West, R. and Krauss, R. Explosives detection using quadrupole resonance analysis. Second Explosives Detection Technology Symposium & Aviation Security Technology Conference, Atlantic City, NJ, 1996, pp. 275-280.
284. Rayner, T., Burnett, L. and West, R. Performance trade-offs in quadrupole resonance analysis screening. Second Explosives Detection Technology Symposium & Aviation Security Technology Conference, Atlantic City, NJ, 1996, pp. 287-292.
285. Krauss, R. A. Development testing of a quadrupole resonance explosives detection device. Second Explosives Detection Technology Symposium & Aviation Security Technology Conference, Atlantic City, NJ, 1996, pp. 281-286.
286. Grechishkin, V. S. NQR device for detecting plastic explosives, mines and drugs. Applied Physics A, 1992, 55, 505-507.
287. Rudakov, T. N., Mikhaltsevich, V. T. and Selchikhin, O. P. The use of multipulse nuclear quadrupole resonance techniques for the detection of explosives containing RDX. Journal of Physics D: Applied Physics, 1997, 30, 1377-1382.
288. Rayner, T. J., Hibbs, A. and Burnett, L. J. Quadrupole resonance explosive detection systems. Sixth International Symposium on Analysis and Detection of Explosives, Prague, Czech Republic, 1998.

2.2.1.6 Microwave spectroscopy

Concept

Microwave spectra of test samples is obtained by illuminating the sample with microwave radiation of varying wavelength and detecting the amount of backscattered radiation. Absorption and resonance bands as well as the general scattering intensity, provide information on the composition of the sample. Optical interferences caused by physical size resonances can distort

the spectra. Imaging is available using mechanical motion for the azimuthal direction, frequency-swept or pulsed illumination for range, and a receiver array for the elevation coordinate.

Demonstrated materials with associated detection limits and matrix effects

Ammonium sulfate box, 2 lb. Imaged in a soft-sided suitcase.

Applicable References

289. Falconer, D. G. and Watters, D. G. Explosive detection using microwave imaging. First International Symposium on Explosive Detection Technology, Atlantic City, NJ, 1991, pp. 486-492.

2.2.1.7 Millimeter wave imaging

Concept

Millimeter wavelength radiation penetrates many optically opaque materials such as clothing. They are usually reflected by metals and the human body, but dielectric materials such as plastics, ceramics and organic materials, partially reflect the waves and appear partially transparent. An imaging system using millimeter waves has been constructed to detect concealed explosives.

Applicable References

290. Sheen, D. M., McMakin, D. L., Collins, H. D., Hall, T. E. and Severtsen, R. H. Concealed explosive detection on personnel using a wideband holographic millimeter-wave imaging system. Conference on Signal Processing, Sensor Fusion, and Target Recognition V, Orlando, FL, 1996. SPIE Proceedings, 1996, 2755, 503-513.

2.2.1.8 Terahertz imaging

Concept

The first use of terahertz radiation to image objects was achieved by Wu and Nuss. The intensity and phase of a terahertz beam was measured while the object was scanned in the two dimensions orthogonal to the beam, because only a single detector element was used. Recently, free space electro-optic sampling has been used to provide real-time coherent 2D imaging of a terahertz beam, making real-time imaging more of a reality. At each point in the image the signal depends on the time-dependent dielectric function of the sample. Variations in material or density cause variations in the signal at each point. Depth information is provided by time resolution. As this methodology matures, there will likely be many applications to detection of concealed explosives, but none could be found in the literature to date.

Applicable References

291. B. B. Wu and M. C. Nuss, 1995. Opt. Lett. **20**, 1716

2.2.1.9 Dielectric sensor methods

Concept

Many materials have unique dielectric constants and dissipation factors. For example, air has a dielectric constant near 1 and a dissipation factor near zero and will not absorb microwave energy. The effect has been incorporated in a portal design, which has a sensor with an antenna lens combination that establishes a fixed field of microwave energy at 5.5 GHz. Objects that enter the field alter it. The microwave energy penetrates nonmetallic objects and produces a volumetric reflection coefficient, which allows calculation of the dielectric constant and dissipation factor. The portal is able to detect concealed devices and say whether they are metal or something like plastic, but not the chemical composition.

Applicable References

292. Seward, D. C. and Yukl, T. Explosive detection using dielectrometry. First International Symposium on Explosive Detection Technology, Atlantic City, NJ, 1991, pp. 441-453.
293. Seward, C. and Yukl, T. Dielectric portal for screening people. Second Explosives Detection Technology Symposium & Aviation Security Technology Conference, Atlantic City, NJ, 1996, pp. 162-169.

2.2.1.10 Raman spectroscopy

Concept

Raman scattering occurs because of the inelastic scattering of light from molecules or atoms. During the interaction of the primary light quantum with a molecule or crystal, the energy of vibrational and/or rotational states may be exchanged and a secondary light quantum of lower or higher energy is emitted. The energy difference is equal to the *vibrational energy* E_{vib} of a molecule or crystal and/or the *rotational energy* E_{rot} of a molecule. It may be recorded, if monochromatic radiation is used for the primary excitation, as a *vibrational, rotational or rotation vibration Raman spectrum*. The inelastic interaction of a primary light quantum with a molecule or crystal in its rotational or vibrational ground state produces the *Stokes Raman spectrum*, a red-shifted spectrum. Due to thermal excitation according to the Boltzmann equation, some molecules are in their vibrational (or rotational) excited states. The interaction of the primary light with these molecules may produce a blue-shifted Raman spectrum, the *anti-Stokes Raman spectrum*. The relative intensity of the Raman lines in the Stokes and anti-Stokes Raman spectra may be employed using the Boltzmann equation for the determination of the *vibrational (or rotational) temperature*.

Raman spectrometers for detection of explosives have been of the dispersive type with CCD detection, and of the Fourier-transform type with excitation at 1064 nm and a near infrared detector. The use of the reddest excitation possible minimizes complications due to sample fluorescence. However, sample heating can be a problem because of the usual compensation for the $1/\lambda^4$ scattering cross section dependence on wavelength requiring larger excitation energies at 1064 nm. The dispersive/CCD type Raman instruments have been made quite portable (< 10 kg

total weight) facilitating field use. Fluorescence interferences and the extremely weak nature of the Raman effect make the use of Raman for trace detection of explosives problematic unless resonance or surface enhancement methods are used.

Raman has been used successfully to detect residual explosives in fingerprint samples. An attempt to do similarly to detect residual explosives in a fingerprint on a cardboard box was unsuccessful because of the enormous fluorescence signal from the cardboard.

Demonstrated materials with associated detection limits and matrix effects

TATB: 0.1% (mass) in soil (Moore)

Applicable References

294. Moore DS, 2001. Fresenius J Anal Chem 369 :393–396
295. Gupta N, Dahmani R, Spectrochimica Acta Part A 56 (2000) 1453–1456
296. McNesby KL, Coffey CS. 1997. *J. Phys. Chem. B* 101:3097–104
297. Fell NF, Widder JM, Medlin SV, Morris JB, Pesce-Rodriguez RA, McNesby KL. 1996. *J. Raman Spectrosc.* 27:97–104
298. Lewis, I. R., Daniel, Jr., N. W., Chaffin, N. C., Griffiths, P. R. and Tungol, M. W. Raman spectroscopic studies of explosive materials: towards a fieldable explosives detector. *Spectrochimica Acta Part A*, 1995, 51, 1985-2000.
299. Cheng C, Kirkbride TE, Batchelder DN, Lacey RJ, Sheldon TG. 1995. *J. Forensic Sci.* 40(1):31–37
300. Hayward IP, Kirkbride TE, Batchelder DN, Lacey RJ. 1995. *J. Forensic Sci.* 40(5):883–84
301. Kneipp K, Wang Y, Dasari RR, Feld MS, Gilbert BD, 1995. *Spectrochim. Acta* 51A:2171–75
302. Lacey RJ. 1995. *IEE Conf. Publ.* 408:138–41
303. Mercado A, Janni J, Gilbert B. 1995. *SPIE Proc.* 2511:142–52
304. Cheng, C., Kirkbride, I. E., Batchelder, D. N., Lacey, R. J. and Sheldon, T. G. In situ detection and identification of trace explosives by Raman microscopy. *Journal of Forensic Sciences*, 1995, 40, 31-37.
305. Hayward, I. P., Kirkbride, T. E., Batchelder, D. N. and Lacey, R. J. Use of fiber optic probe for the detection and identification of explosive materials by Raman spectroscopy. *Journal of Forensic Sciences*, 1995, 40, 883-884.
306. McNesby KL, Wolfe JE, Morris JB, Pesce-Rodriguez RA. 1994. *J. Raman Spectrosc.* 25:77–87
307. Carver FWS, Sinclair TF. 1983. *J. Raman Spectrosc.* 14:470–74
308. Akhavan J. 1991. *Spectrochim. Acta* 47A:1247–50
309. Hendra P, ed. 1990. *Spectrochim. Acta* 46A:121–337

310. Coithup, N. B. Infrared and Raman spectroscopy. In: Gouw T. H. (ed.), Guide to Modern Methods of Instrumental Analysis, Wiley-Interscience, New York, 1972, pp. 195-229.

2.2.2. Neutron techniques

Concept

Active neutron interrogation techniques are based on the interactions of neutrons with individual atoms in the investigated object. Neutrons are highly penetrating probes that generate distinguishable and detectable reaction products from the different elements constituting the various substances present. The key elements of a neutron based method are a neutron source, a neutron moderator and/or collimator, a means of detection and the data processing. The excited atoms react in different ways, but usually emit detectable characteristic radiation such as γ rays. The methods can be categorized as: thermal neutron analysis (TNA), fast neutron analysis (FNA), pulsed fast neutron analysis (PFNA), pulse fast-thermal neutron analysis (PFTNA), fast neutron transmission spectroscopy (FNTS), gamma-to-fast neutron ratio analysis (GFNA), neutron elastic scatter (NES), and associated particle imaging (API). Those methods that have been applied to explosives detection are discussed below.

Applicable references

311. Kiraly B, Olah L, Csikai J 2001. Neutron-based techniques for detection of explosives and drugs. Rad. Phys. Chem. 61:781-784.
312. Hussein, E. M. A. Detection of explosive materials using nuclear radiation: a critical review. Conference on Aviation Security Problems and Related Technologies: Critical Reviews, San Diego, CA, 1992, pp. 126-136.
313. Gozani, T. and Shea, P. M. Nuclear based explosive detection systems-1992 status. In: Yinon J. (ed.) Advances in Analysis and Detection of Explosives, Kluwer Academic Publishers, Dordrecht, 1993, pp. 335-349.

2.2.2.1 Thermal neutron activation

Concept

A thermal neutron flux impinges on the investigated object, leading to capture by various atoms and formation of a metastable compound nucleus. If the excited nucleus decays promptly (i.e., in ps timescales), then the emission is useful for these applications. Thermal neutron activation of nitrogen is followed promptly by the emission of a 10.8 MeV γ photon. The γ emission spectrum shows features characteristic of certain types of material. A three dimensional image of the nitrogen characteristic emission can be constructed algorithmically, which can then be used to differentiate between common nitrogen containing materials and those of high density, which are more likely to be explosives.

Applicable References

314. Farsoni AT, Miresghhi SA 2001. Design and evaluation of a TNA explosive-detection system to screen carry-on luggage. J. Radioanal. Nucl. Chem. 248: 695-697
315. da Silva AX, Crispim VR 2001. Use of thermal neutron tomography for the detection of drugs and explosives. Rad. Phys. Chem. 61: 767-769.
316. Gozani, T., Morgado, R. E. and Seher, C. C. Nuclear-based techniques for explosive detection. Journal of Energetic Materials, 1986, 4, 377-414.
317. Gozani, T., Seher, C. C. and Morgado, R. E. Nuclear-based techniques for explosive detection. Third International Symposium on Analysis and Detection of Explosives, Mannheim-Neuostheim, Germany, 1989, pp. 36.31-36.19.
318. Shea, P., Gozani, T. and Bozorgmanesh, H. A TNA explosives-detection system in airline baggage. Nuclear Instruments and Methods in Physics Research A, 1990, 299, 444 -448.
319. Seher, C. C. Airport tests of federal aviation administration thermal neutron activation explosive detection systems. Third International Symposium on Analysis and Detection of Explosives, Mannheim-Neuostheim, Germany, 1989, pp. 34.31-34.11.
320. Caifrey, A. J., Cole, J. D., Gehrke, R. I. and Greenwood, R. C. Chemical warfare agent and high explosive identification by spectroscopy of neutron-induced gamma rays. IEEE Transactions in Nuclear Science, 1992, 39, 1422-1426.

2.2.2.2 Fast neutron activation

Concept

Thermal neutron analysis is relevant for nitrogen and hydrogen, but fast neutron activation is needed to detect carbon and oxygen. The neutrons must have energies above the excitable nuclear levels of the interacting nuclei for γ rays to be stimulated. For carbon and oxygen, neutron energies must be above 5 and 7 MeV, respectively. The detectable γ rays are produced via $(n,n'\gamma)$ reactions. FNA is limited to relatively small objects because larger objects result in a lack of geometrical definition, due to the large distance between inner voxels and the detectors.

Applicable References

321. James WD 2000. 14 MeV fast neutron activation analysis in the year 2000. J. Radioanal. Nucl. Chem. 243:119-123
322. Gozani, T. Novel applications of fast neutron interrogation methods. Nuclear Instruments and Methods in Physics Research A, 1994, 353, 635-640.

2.2.2.3 Pulsed fast thermal neutron analysis

Concept

The advantages of fast versus thermal neutrons to detect carbon and oxygen versus nitrogen are exploited in PFTNA. The fast and thermal neutrons are produced from a pulsed sealed tube neutron generator with and without moderation, respectively.

Applicable References

323. Vourvopoulos G, Womble PC 2001. Pulsed fast/thermal neutron analysis: a technique for explosives detection. *Talanta* 54:459-468
324. Vourvopoulos, G. and Schultz, F. J. A pulsed fast-thermal neutron system for the detection of hidden explosives. *Nuclear Instruments and Methods in Physics Research B*, 1993, 79, 585-588.

2.2.2.4 Pulsed fast neutron analysis

Concept

PFNA combines in-beam γ -ray spectroscopy and neutron time of flight. It utilizes known isotopic cross sections for excitation to specific levels that decay by emitting discrete γ -rays to determine the amount of the specific isotope in the material of interest. The location of that specific isotope is determined by measuring the monoenergetic neutron TOF from its point of creation to the point of interaction with the tested item. The time of prompt γ -ray emission is measured by a NaI γ -ray detector observing orthogonally to the neutron beam. The neutrons must be monoenergetic to prevent faster neutrons from interfering with the γ -rays stimulated by slower neutrons. Signature γ -rays for carbon and oxygen are 4.44 and 6.13 MeV respectively, and for nitrogen 1.63, 2.3 and 5.1 MeV.

Applicable References

325. Sawa, Z. P. PFN GASCA technique for detection of explosives and drugs. *Nuclear Instruments and Methods in Physics Research B*, 1993, 79, 593-596.
326. Gozani, T. Understanding the physics limitations of PFNA - the nanosecond pulsed fast neutron analysis. *Nuclear Instruments and Methods in Physics Research B*, 1995, 99, 743-747.
327. Stevenson, J., Clayton, J., Fankhauser, K., Gozani, T., Jeppesen, R., Liu, F., Merics, T. and Bell, C. PFNA detection of small explosives. 13th International Conference on Applications of Accelerators in Research and Industry, Denton, TX, 1994.

2.2.2.5 Fast neutron transmission spectroscopy

Concept

FNTS is based on the variation of neutron absorption cross sections of carbon, nitrogen, and oxygen nuclei with neutron energy. Usually accelerator methods are used to produce short neutron pulses and time of flight (TOF) techniques are used to measure the transmission as a function of neutron energy. Volume imaging of objects has been achieved using FNTS by laminographic image reconstruction.

Demonstrated materials with associated detection limits and matrix effects

A 400 g TNT object inside a suitcase was imaged at 450 suitcases per hour data rate (Loveman et al)

Applicable References

328. Fink, C. L., Mieldich, B. J., Yule, T. J., Humm, P., Sagalovsky, L. and Martin, M. M. Evaluation of neutron techniques for illicit substance detection. Nuclear Instruments and Methods in Physics Research B, 1995, 99, 748-752.
329. Lefevre, H. W., Rasmussen, R. J., Chmelik, M. S., Schofield, R. M. S., Sieger, G. E. and Overley, J. C. Using a fast-neutron spectrometer system to candle luggage for hidden explosives. International Conference on Neutrons in Research and Industry, Crete, Greece, 1996. SPIE Proceedings, 1997, 2867, 206-210.
330. Loveman, R. A., Feinstein, R. L., Bendahan, J., Gozani, T. and Shea, P. Laminography using resonant neutron attenuation for detection of drugs and explosives. In: Duggan I. L. and Morgan, I. L. (eds.), Application of Accelerators in Research and Industry, Vol. 392, American Institute of Physics, Denton, TX, 1997, pp. 895-898.
331. Gokhale, P. P. and Hussein, E. M. A. A ^{252}Cf neutron transmission technique for bulk detection of explosives. Applied Radiation and Isotopes, 1997, 48, 973-979.

2.2.2.6 Ratio of gamma/neutron transmissions*Concept*

Measurement of the ratio of γ ray to fast neutron attenuation ratios can allow determination of the average atomic number of heterogeneous mixtures. Both the prompt γ ray and neutron attenuations are evaluated from neutron TOF spectra.

Applicable References

332. Dokhale PA, Csikai J, Olah L 2001. Investigations on neutron-induced prompt gamma ray analysis of bulk samples. Applied Radiation and Isotopes 54: 967-971
333. Rasmussen, R. J., Fanselow, W. S., Lefevre, H. W., Chmelik, M. S., Overley, J. C., Brown, A. P., Sieger, G. E. and Schofield, R. M. S. Average atomic number of heterogeneous mixtures from the ratio of gamma to fast-neutron attenuation. Nuclear Instruments and Methods in Physics Research B, 1997, 124, 611-614.

2.2.2.7 Neutron elastic scattering*Concept*

Neutron elastic scatter includes both neutron resonant elastic scatter and neutron elastic back scatter. Use of NES to detect and locate conceal explosives is based on measurement of carbon nitrogen and oxygen contents and calculation of carbon-nitrogen and oxygen-nitrogen ratios, which fall into a narrow range for common explosives. In elastic collisions, there is no change in the structure of the nucleus hit by the neutron, but the neutrons scattered in a certain direction have a new and unique reduced energy determined by the mass of the nucleus hit. The reduced energy spectrum is measured using TOF. The intensity versus energy reveals the amounts of each chemical element in the probed object.

Applicable References

- 334. Buffler A, Brooks FD, Allie MS, Bharuth-Ram K, Nchodu MR 2001. Material classification by fast neutron scattering. Nucl. Instr. & Meth. In Phys. Res. B 173:483-502.
- 335. Gomberg, H. J. and Kushner, B. G. Neutron elastic scatter (NES) for explosives detection systems (EDS). First International Symposium on Explosive Detection Technology, Atlantic City, NJ, 1991, pp. 123-139.

2.2.2.8 Associated particle imaging

Concept

The API technique uses the direction and time correlation between 14.1 MeV neutrons and alpha particles produced in a small accelerator via the deuterium-tritium reaction. The alpha particles are detected with a position sensitive detector to provide direction of flight and time of emission of the associated neutron. The direction and subsequent interaction point of the neutron (and therefore the spatial location of the target materials) can be determined by the time of detection of the γ ray, while measurement of the γ ray energy identifies the elemental composition of the target. Neutron production rate must be kept low enough to limit random coincidences, which disguise which neutron produced the detected γ ray, which limits data rates and therefore sample throughput.

Applicable References

- 336. Beyerle, A., Hurley, J. P. and Tunnell, L. Design of an associated particle imaging system. Nuclear Instruments and Methods in Physics Research A, 1990, 299, 458-462.
- 337. Beyerle, A., Durkee, R., Headley, G., Hurley, J. P. and Tunnell, L. Associated particle imaging. First International Symposium on Explosive Detection Technology, Atlantic City, NJ, 1991, pp. 160-174.

2.3 Detection of degradation products

2.3.1 Degradation products

Concept

Explosives degrade over time in storage and in the environment. The environmental concerns about explosives center on toxicology of the explosive itself and its degradation products, which has driven the development of many sensitive detection methods. Degradation processes include photochemistry, thermal cycling, and biotransformation.

Applicable References

338. Adrian NR, Chow T, 2001. Identification of hydroxylamino-dinitroso-1,3,5-triazine as a transient intermediate formed during the anaerobic biodegradation of hexahydro-1,3,5-trinitro-1,3,5-triazine. *Env. Tox. Chem.* 20: 1874-77
339. Yinon, J., Zitrin, S. and Tamiri, T. Reactions in the mass spectrometry of 2,4,6-N-tetranitro-N-methylaniline (tetryl). *Rapid Communications in Mass Spectrometry*, 1993, 7, 1051-1054.
340. Walsh, M. E. Environmental transformation products of nitroaromatics and nitramines. Special Report No. 90-2 (ADA220-610), U.S. Army Cold Regions Research and Engineering Laboratory, Hanover, NH, 1990.
341. Basch, A., Margalit, Y., Abramovich-Bar, S., Bamberger, Y., Daphna, D., Tamiri, T. and Zitrin, S. Decomposition products of PETN in post explosion analysis. *Journal of Energetic Materials*, 1986, 4, 77-91.
342. Tamiri, T. and Zitrin, S. Capillary column gas chromatography/mass spectrometry of explosives. *Journal of Energetic Materials*, 1986, 4, 215-237.
343. Kaplan, D. L. and Kaplan, A. M. Thermophilic biotransformation of 2,4,6-trinitrotoluene under simulated composting conditions. *Applied and Environmental Microbiology*, 1982, 44, 757-760.
344. Burlinson, N. E., Kaplan, L. A. and Adams, C. E. Photochemistry of TNT: investigation of the pink water' problem. Report No. NOLTR73-172 (AD-76970), Naval Ordnance Laboratory, White Oak, Silver Spring, MD, 1973.
345. McCormick, N. O., Feeherry, F. E. and Levinson, H. S. Microbial transformation of 2,4,6-trinitrotoluene and other nitroaromatic compounds. *Applied and Environmental Microbiology*, 1976, 31, 949-958.
346. Farey, M. G. and Wilson, S. E. Quantitative determination of tetryl and its degradation products by high-pressure liquid chromatography. *Journal of Chromatography*, 1975, 114, 261-265.
347. Kayser, E. G., Burlinson, N. E. and Rosenblatt, D. H. Kinetics of hydrolysis and products of hydrolysis and photolysis of tetryl. Technical Report No. 84-78 (ADA 153144), Naval Surface Weapons Center, Silver Spring, MD, 1984.
348. Yasuda, S. K. Separation and identification of tetryl and related compounds by two-dimensional thin-layer chromatography. *Journal of Chromatography*, 1970, 50, 453-457.
349. McCormick, N. G., Cornell, J. H. and Kaplan, A. M. Biodegradation of hexa-hydro- 1,3,5-trinitro-1,3,5-triazine. *Applied and Environmental Microbiology*, 1981, 42, 817-823.

350. Patterson, J., Shapira, N. I., Brown, J., Duckert, W. and Poison, J. State-of-the-art: Military explosives and propellants production industry. Vol 2. Report No. 600/2-76-213b, American Defense Preparedness Association, Washington, DC, 1976.
351. Wendt, T. M., Cornell, J. H. and Kaplan, A. M. Microbial degradation of glycerol nitrates. Applied and Environmental Microbiology, 1978, 36, 693-699.

2.3.2 Chemical color sensors

Concept

Several kinds of color change chemical sensors have been developed for rapid on-site detection of explosives and their impurities and/or degradation products. The reagents to produce the colored adduct have been contained in exchange resin matrices, polymeric membranes, and porous thin films which are incorporated into various fieldable devices. The color change has been recorded visually or with fiber optic based UV/visible absorption spectrometry or fluorescence quenching methods. Color reactions have also been developed for soil contamination screening methods.

Demonstrated materials with associated detection limits and matrix effects

TNT: 100 ppb in water (Heller et al.)

TNT and DNT: 2 mg/L; RDX: 10 mg/L (Jian and Seitz)

Applicable References

352. Arbuthnot, D., Bartholomew, D. U., Carr, R., Elkind, J. L., Gheorghiu, L., Melendez, J. L. and Seitz, W. R. Detection of a polynitroaromatic compound using a novel polymer-based multiplate sensor. Conference on Detection and Remediation Technologies for Mines and Minelike Targets III, Orlando, FL, 1998. SPIE Proceedings, 1998, 3392, 432-440.
353. Medary, R. T. Inexpensive, rapid field screening test for 2,4,6-trinitrotoluene in soil. Analytica Chimica Acta, 1992, 258, 341-346.
354. Jenkins, T. F. and Walsh, M. E. Development of field screening methods for TNT, 2,4-DNT and RDX in soil. Talanta, 1992, 39, 419-428.
355. Jian, C. and Seitz, W. R. Membrane for in situ optical detection of organic nitro compounds based on fluorescence quenching. Analytica Chimica Acta, 1990, 237, 265-271.
356. Stevanovic, S. and Mitrovic, M. Colorimetric method for semiquantitative determination of nitroorganics in water. International Journal of Environmental Analytical Chemistry, 1990, 40, 69-76.
357. Zhang, Y., Seitz, W. R. and Grant, C. L. A clear, amine-containing poly(vinyl chloride) membrane for in situ optical detection of 2,4,6-trinitrotoluene. Analytica Chimica Acta, 1989, 217, 217-227.

358. Zhang, Y., Seitz, W. R., Sundberg, D. C. and Grant, C. L. Preliminary development of a fiber optic sensor for TNT. Special Report No. 88-4, U.S. Army Cold Regions Research and Engineering Laboratory, Hanover, NH, 1988.
359. Zhang, Y. and Seitz, W. R. Single fiber absorption measurements for remote detection of 2,4,6-trinitrotoluene. *Analytica Chimica Acta*, 1989, 221, 1-9.
360. Heller, C. A., Greni, S. R. and Erickson, E. D. Field detection of 2,4,6-trinitrotoluene in water by ion-exchange resins. *Analytical Chemistry*, 1982, 54, 286-289.

2.3.3 Immunochemical sensors

Concept

Antigen-antibody complexes can be formed for proteins containing a molecule of interest (explosive). When the substance binds to the antibody a change in a physical property (e.g., absorption or fluorescence) can occur, which leads to a method of detection. Usually these immunosensors are operated under continuous flow conditions. Sometimes materials (usually plastic beads) containing the antibodies have been previously treated with a fluorescent dye-labeled explosive analog that is released to the solution when the explosive interacts with the antibody (referred to as competitive immunoassay). One commonly used method is the enzyme-linked immunosorbent assay (ELISA). ELISA is based on the specificity of the antibody for the analyte and the resultant immune complex. The main development for application to explosives is deriving analyte specific antibodies, to maximize the specificity and sensitivity for each target compound. Immunochemical sensors can have incredible detection limits, sometimes in the ng/L range.

During the last decade, the continuous flow displacement immunosensor (CFI) has emerged as a rapid, sensitive, and portable assay format for the detection of explosives (Whelan et al., 1993; Bart et al., 1997). While similar to affinity chromatographic techniques, there is an important distinction. The performance of a displacement assay is heavily dependent on the dissociation kinetics between the labeled analyte and immobilized antibodies. CFIs offer certain advantages over competing technologies in low or medium throughput screening scenarios. After the initial preparation of the sensor, it is reagentless: there are no secondary reagents and incubation periods after sample injection. This leads to typical response times of less than 2 min.

Demonstrated materials with associated detection limits and matrix effects

Competitive fluorescent immunoassay	TNT and RDX 5 $\mu\text{g/L}$ (VanBergen et al.)
ELISA	TNT: 20 ng/L (Niessner et al. 1992)

Applicable References

361. Holt DB, Gauger PR, Kusterbeck AW, Ligler FS. 2002. Fabrication of a capillary immunosensors in polymethyl methacrylate. *Bios. Bioelec.* 17: 95-103.
362. Goldman ER, Pazirandeh MP, Charles PT, Balighian ED, Anderson GP. 2002. Selection of phage displayed peptides for the detection of 2,4,6-trinitrotoluene in seawater. *Anal. Chim. Acta.* 457: 13-19

363. Altstein M, Bronshtein A, Glattstein B, Zeichner A, Tamiri T, Almog J. 2001. Immunochemical approaches for purification and detection of TNT traces by antibodies entrapped in a sol-gel matrix. *Anal. Chem.* 73: 2461-2467.
364. Shriver-Lake LC, Patterson CH, Van Bergen SK, 2000. New horizons: Explosive detection in soil extracts with a fiber-optic biosensor. *Field Anal. Chem. Tech.* 4: 239-245
365. VanBergen SK, Bakaltcheva IB, Lundgren JS, Shriver-Lake LC, 2000. *Environ. Sci. Technol.* 34:704-708
366. Zeck A, Weller MG, Niessner R 1999. Characterization of a monoclonal TNT-antibody by measurement of the cross-reactivities of nitroaromatic compounds. *Fresenius J. Anal. Chem* 364: 113-120
367. Bart JC, Judd LL, Hoffman KE, Wilkins AM, Kusterbeck AW. 1997. *Environ. Sci. Technol.* 31:1505-11
368. Bart, J. C., Judd, L. L., Hoffman, K. E., Wilkins, A. M. and Kusterbeck, A. W. Application of a portable immunosensor to detect the explosives TNT and RDX in groundwater samples. *Environmental Science & Technology*, 1997, 31, 1505-1511.
369. Bart, J. C., Judd, L. L. and Kusterbeck, A. W., Environmental immunoassay for the explosive RDX using a fluorescent dye-labeled antigen and the continuous-flow immunosensor. *Sensors and Actuators B*, 1997, 38-39, 411-418.
370. Shriver-Lake, L. C., Donner, B. L. and Ligler, F. S. On-site detection of TNT with a portable fiber optic biosensor. *Environmental Science & Technology*, 1997, 31, 837-841.
371. Narang, U., Gauger, P. R. and Ligler, F. S. Capillary-based displacement flow immunosensor. *Analytical Chemistry*, 1997, 69, 1961-1964.
372. Narang, U., Gauger, P. R. and Ligler, F. S. A displacement flow immunosensor for explosive detection using microcapillaries. *Analytical Chemistry*, 1997, 69, 2779-2785.
373. Judd LL, Kusterbeck AW, Conrad DW, Yu H, Myles HL Jr, Ligler FS. 1995. *SPIE Proc.* 2388:198-204
374. Shriver-Lake LC, Breslin KA, Golden JP, Judd LL, Choi J, Ligler FS. 1995. *SPIE Proc.* 2367:52-58
375. Lukens HR. 1992. In: *Proc. Int. Symp. Explosive Detection Technology, 1st*. Atlantic City: FAA, pp. 753-58
376. Bart, J. C., Judd, L. L., Hoffman, K. E., Wilkins, A. M., Charles, P. T. and Kusterbeck, A. W. Detection and quantitation of the explosives TNT and RDX in groundwater using a continuous flow immunosensor. In: Aga D. S. and Thurman E. M. (eds), *Development and Applications of Immunoassays for Environmental Analysis*, ACS symposium Series, Vol. 657, American Chemical Society, Washington. D., 1996, pp. 210-220.
377. Anon. TNT RaPID Assay, Product file, Strategic Diagnostics, Inc., Newark, DE, 1995.

378. Shriver-Lake, L. C., Breslin, K. A., Charles, P. T., Conrad, D. W., Golden, J. P. and Ligler, F. S. Detection of TNT in water using an evanescent wave fiber-optic biosensor. *Analytical Chemistry*, 1995, 67, 2431-2435.
379. Kusterbeck W, Judd LL, Yu H, Myles J, Ligler FS. 1994. *SPIE Proc.* 2092:218–26
380. Whelan JP, Kusterbeck AW, Wemhoff GA, Bredehorst R, Ligler FS. 1993. *Anal. Chem.* 65:3561–65
382. Van Emon, J. M. and Lopez-Avila, V. Immunochemical methods for environmental analysis. *Analytical Chemistry*, 1992, 64, 78A-88A.
383. Keuchel, C. and Niessner, R. Rapid field screening test for determination of 2,4,6-trinitrotoluene in water and soil with immunofiltration. *Fresenius Journal of Analytical Chemistry*, 1994, 350, 538-543.
383. Keuchel, C., Weil, L. and Niessner, R. Enzyme-linked immunosorbant assay for the determination of 2,4,6-trinitrotoluene and related nitroaromatic compounds. *Analytical Sciences*, 1992, 8, 9-12.
384. Keuchel, C., Weil, L. and Niessner, R. Effect of the variation of the length of the spacer in a competitive enzyme immunoassay (ELISA) for the determination of 2,4,6-trinitrotoluene (TNT). *Fresenius Journal of Analytical Chemistry*, 1992, 343, 143-143.
385. Eck, D. L., Kurth, M. J. and Macmillan, C. Trinitrotoluene and other nitroaromatic compounds-Immunoassay methods. In: Van Emon J. M. and Mumma R. O. (eds.), *Immunochemical Methods for Environmental Analysis*, ACS Symposium Series, Vol. 442, Chapter 9, American Chemical Society, Washington, DC, 1990, pp. 79-94.
386. Bhatia, S. K., Shriver-Lake, L. C., Prior, K. J., Georger, J. H., Calvert, J. M., Bredehorst, R. and Ligler, F. S. Use of thiol-terminal silanes and heterobifunctional crosslinkers for immobilization of antibodies on silica surfaces. *Analytical Biochemistry*, 1989, 178, 408-413.
387. Whelan, J. P., Kusterbeck, A. W., Wemhoff, G. A., Bredehorst, R. and Ligler, F. S. Continuous-flow immunosensor for detection of explosives. *Analytical Chemistry*, 1993, 65, 3561-3565.

2.3.4 Electrochemical sensors

Concept

Electroanalytical methods include voltammetry [$i \neq 0$; $E = f(t)$], potentiometry ($i = 0$), amperometry ($i \neq 0$; $E = \text{const}$), impedance or conductance, and combinations. Electrochemical cells can be divided into two classes: galvanic and electrolytic. Galvanic cells can operate continuously because the opposing electromotive force (emf) is absolutely less than the zero current potentiometric potential difference. Chemical energy is converted into electrical energy. The open circuit emf is the limiting value of the electric potential difference at zero current. An electrolytic cell is one in which chemical reactions are caused by applying an external potential difference (E) greater than, and opposite to, the galvanic emf of the cell. The zero current emf lies numerically between the decreasing cell potential differences during galvanic action, and the absolutely larger applied potential differences required for electrolytic action.

Methods used for detection of explosives are amperometry (TNT thermal degradation products – Buttner et al.), cyclic voltammetry (TNT in environmental samples – Krausa et al.), and square wave voltammetry (TNT in water – Wang et al.) including disposable sensors.

Wang et al. have also utilized a variety of electrochemical detection schemes as detectors for capillary electrophoresis or other separation methods on a chip. Chip based methods have grown rapidly in importance, because of the increase in detection speed as well as their ability to be used *in situ* or in the field.

Demonstrated materials with associated detection limits and matrix effects

Square wave voltammetry with screen printed disposable carbon electrodes: TNT < 100 ppb (Wang et al. 1998); Interferences possible from other explosives as well as fertilizers.

Applicable References

388. Wang J, Pumera M, 2002. Dual conductivity/amperometric detection system for microchip capillary electrophoresis. *Anal. Chem.* 74: 5919-5923
389. Wang J, Pumera M, Chatrathi MP, Escarpa A, Musameh M, 2002. Single-channel microchip for fast screening and detailed identification of nitroaromatic explosives or organophosphate nerve agents. *Anal. Chem.* 74: 1187-+
390. Lu Q, Collins GE, Smith M, Wang J, 2002. Sensitive capillary electrophoresis microchip determination of trinitroaromatic explosives in nonaqueous electrolyte following solid phase extraction. *Analytical Chimica Acta* 469: 253-260
391. Hilmi A, Luong JHT, 2000. Micromachined electrophoresis chips with electrochemical detectors for analysis of explosive compounds in soil and groundwater. *Env. Sci. Tech.* 34: 3046-3050.
392. Wang J, Tian BM, Sahlin E, 1999. Micromachined electrophoresis chips with thick-film electrochemical detectors. *Anal. Chem.* 71: 5436-5440
393. Wang, J., Bhada, R. K., Lu, J. and McDonald, D. Remote electrochemical sensor for monitoring TNT in natural waters, *Analytica Chimica Acta*, 1998, 361, 85-91.
394. Wang, J., Lu, F., MacDonald, D., Lu, J., Ozsoz, M. E. S. and Rogers, K. R. Screen-printed voltammetric sensor for TNT. *Talanta*, 1998, 46, 1405-1412.
395. Buttner, W. J., Findlay, M., Vickers, W., Davis, W. M., Cespedes, E. R., Cooper, S. and Adams, J. W. In situ detection of trinitrotoluene and other nitrated explosives in soils. *Analytica Chimica Acta*, 1997, 341, 63-71.
396. Wormhoudt, J., Shorter, J. H. and Kolb, C. E. Mechanisms underlying the cone penetrometer detection of energetic materials in soils. Conference on Field Analytical Methods for Hazardous Wastes and Toxic Chemicals, Las Vegas, NV, 1997.
397. Krausa, M., Doll, J., Schorb, K., Boke, W. and Hambitzer, G. Fast electrochemical detection of nitro- and aminoaromatics in soils and liquids. *Propellants, Explosives, Pyrotechnics*, 1997, 22, 156-159.

398. Wormhoudt, J., Shorter, J. H., McManus, J. B., Kebabian, P. L., Zahniser, M. S., Davis, W. M., Cespedes, E. R. and Kolb, C. E. Tunable infrared laser detection of pyrolysis products of explosives in soils. *Applied Optics*, 1996, 35:3992-3997.
399. Cao, Z., Buttner, W. J. and Stetter, J. R. The properties and applications of amperometric gas sensors. *Electroanalysis*, 1992, 4, 253-266.
400. Bard, A. J. and Faulkner, L. R. *Electrochemical Methods. Fundamentals and Applications*, John Wiley & Sons, New York, 1980.

2.3.5 Laser optical sensors

Concept

As discussed above for infrared absorption detection of pyrolysis products, environmental monitors have been developed to detect explosive contamination of soils. The soil sample is heated and the decomposition products collected in a multipass cell. The materials can also be decomposed using photofragmentation by a laser followed by laser induced fluorescence of some of the products such as NO.

Demonstrated materials with associated detection limits and matrix effects

PF-LIF: TNT 40 ppb in soil (Boudreaux et al.). Water quenches fluorescence.
TNT: low ppb (volume) in air (Swayambunathan et al.)

Applicable References

401. Shu J, Bar I, Rosenwaks S. 2000. NO and PO photofragments as trace analyte indicators of nitrocompounds and organophosphonates. *Appl. Phys. B* 71:665-672
402. Swayambunathan V, Sausa RC, Singh G. 2000. Investigations into trace detection of nitrocompounds by one- and two-color laser photofragmentation/fragment detection spectrometry. *Appl. Spectrosc.* 54: 651-658
403. Boudreaux, G. M., Miller, T. S., Kunecke, A. J., Singh, J. P., Yueh, F.-Y. and Monts, D. L. Toward development of a photofragmentation-laser induced fluorescence (PF-LIF) laser sensor for detection of 2,4,6-trinitrotoluene (TNT) in soil and groundwater. *Applied Optics*, 1999, 38, 1411-1417.
404. Wu, D., Singh, J. P., Yueh, F. Y. and Monts, D. L. 2,4,6-Trinitrotoluene detection by laser-photofragmentation-laser-induced fluorescence. *Applied Optics*, 1996, 35,3998-4003.

3 Implemented Detection Systems

The number of systems actually implemented for detection of explosive materials is really quite limited. These can be categorized as luggage screening devices, passenger screening portals, and other testing technologies. There has also been some effort in the qualification and certification protocols for these detection systems. The materials below are therefore categorized into the broad categories: Luggage Screening, Passenger Screening Portals, Other Testing Technologies, and Testing Materials and Methodology. A listing of the web addresses where this information was obtained is given in the last section.

An excellent source for implemented technologies up to 1999 is the National Academies 1999 report <http://books.nap.edu/books/0309067871/html/index.html>. An example of the types of data and analysis is shown in the figure and statement below.

“Keeping bombs off of aircraft is the primary measure of the performance of a TAAS (total architecture for aviation security). Improved security components recently deployed to minimize the probability that a bomb can be placed on an aircraft by a terrorist include CAPS (computer-assisted passenger screening), PPBM (positive passenger-bag matching), HULDS (hardened unit-loading devices), TEDDs (trace explosives-detection devices), non-certified bulk explosives-detection equipment, and EDSs (FAA-certified bulk explosives-detection systems). Blind operational testing using realistic simulated bombs will be necessary to evaluate the effectiveness of the overall aviation security system. At present the FAA has only limited blind-test data on EDSs and even less data on other components of the TAAS. Test results on all TAAS components will be necessary for a systems analysis that can estimate the results of full-scale field testing of the entire TAAS. A sensitive measure of effectiveness, such as the SEF (security enhancement factor), could be used to assess improvements to TAAS components and reduce the complexity of evaluating the whole system.”

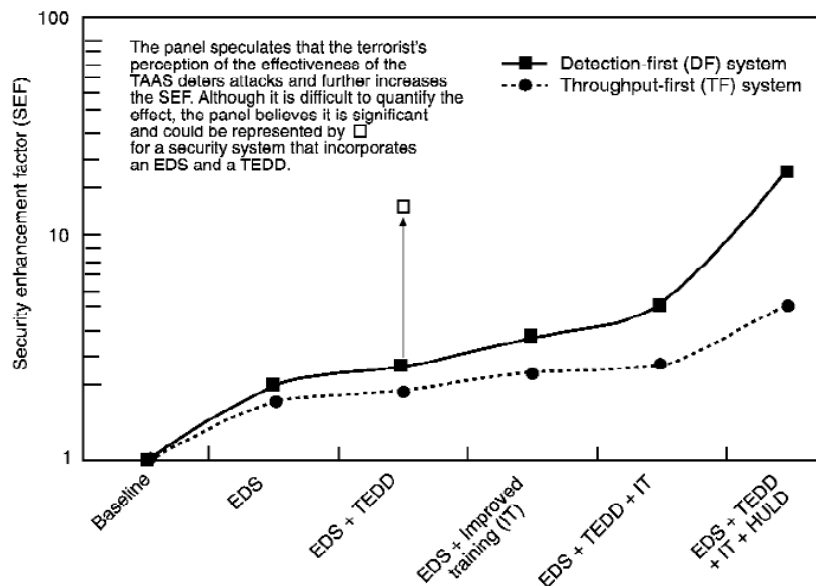


FIGURE 10-1 Comparative contributions (notional) to the SEF of detection-first and throughput-first systems.

In FY 2000, the FAA continued in its mission to develop and deploy products that prevent explosives, weapons, and other threat material from being introduced on to aircraft. Major areas of concentration included certification testing, checked and carry-on baggage screening, using bulk and trace explosives detection, human factors, aircraft hardening, Aviation Security Technology Integration (ASTI), and airport deployment of systems by the security equipment integrated product team. The Aviation Security Laboratory (ASL) conducted certification tests on the InVision CTX 9000Dsi Explosives Detection System (EDS) production unit and the L3 eXaminer 3DX 6000 unit. Both systems passed agency tests. Bulk detection research included additional work in quadrupole resonance and x-ray diffraction techniques. The ASL evaluated 2 new Explosives Trace Detection (ETD) models that are now deployed at over 170 locations. Other activities in FY 2000 included development of quality control standards for deployed ETD systems. As an alternative for EDSs at smaller airports, ASL conducted an evaluation of directed trace. This involves x-ray identification of target items to be directly screened by trace systems. As a follow-on, the ASL initiated the Argus program for the development of a lower-cost EDS. This system would also be automated and have the same performance requirements, except for lower throughput. In the area of personnel screening, three ETD portal prototypes and the evaluation of two bulk detection portals were completed. The ASL evaluated several large cargo inspection systems and a large bulk EDS for break-bulk cargo. The agency also established an explosives standard system (Trace Personnel Standard-Dry Transfer Method) enabling the evaluation of emerging explosives trace detection technology.

FAA Transportation Security Laboratory (TSL): Explosives And Weapons Detection R&D [AAR-520]:

AAR-520 conducts applied research and development (R&D) with principal emphasis on current and emerging aviation security technology targeted at identified operating requirements; conducts technical feasibility demonstrations, analyzes impact, develops concepts, and conducts objective assessments of evolving technologies; and concentrates on the most promising research areas, with the highest technological dividend, through effective national and international scientific cooperation and communications.

The branch maintains a scientific base, a multi-disciplinary perspective, and an eye on the impact of technology change through its cadre of expert scientific and engineering personnel.

The branch is responsible for assisting in the developmental test and evaluation (DT&E) of new and improved security systems developed by the division and support for the independent operational test and evaluation (IOT&E) of completed systems.

The branch is responsible for the development of aviation security technology in all areas of aviation security, including, but not limited to, explosives/weapons detection for checkpoint, baggage, and cargo vectors. These developments lean toward detection methods such as nuclear, electromagnetic, x-ray, and trace technologies. The branch also conducts research and development pertaining to canine detection methodology.

3.1 Passenger Screening Portals

Commercial portals now on the market include the Barringer Sentinel®, the Thermedics Detection SecurScan™, and the Ion Track Industries Entryscan 3™. Each of these portals was developed primarily for the aviation security market, though both the Sentinel® and the Entryscan 3™ advertise the capability to detect CBW agents as well. Of these devices, the Entryscan 3™ and the Sentinel® rely on IMS detectors while the SecurScan™ uses a fast GC with chemiluminescent detection. In terms of physical principles, the Entryscan 3™ takes advantage of the human thermal plume. The SecurScan™ employs physical contact with human subjects using perforated wands that sample a small airflow rate from the intimate vicinity of the human body. The Sentinel® employs twin slot-jets which direct airstreams downward over the body with collection near the floor. All three commercial devices have demonstrated the ability to detect trace explosives on human subjects. Portals such as these can be characterized by varied sensitivity thresholds and false-alarm rates. Each requires a human operator, and in each case the most expensive portal component is the detector.

American Science & Engineering manufacture the BodySearch™, already installed by United States Customs in six airports around America. The system utilizes AS&E patented Z® Backscatter technology, first developed in 1986. This has been particularly useful in respect of X-raying the human body where the intent is to detect items that would not normally be detected by the traditional archway metal detector. Low density materials, such as narcotics and explosives, are identifiable as the Z® Backscatter technology is designed to highlight such low atomic number materials in a separate image.

Sandia National Laboratory: Explosives detection portal uses high flow rate pre-concentrator and IMS; not implemented, but undergoing testing at a variety of locations. “With a \$1 million grant from the FAA, Orange County-based Syagen, working with Sandia Laboratories, has developed a chemical and explosive detection technology to be used at airports.”

Eurotech has developed the Acoustic Core Portal, which utilizes FFT of acoustic impedance spectral signatures. Information about the technology can be obtained at: <http://www.eurotechltd.com/products/nets/acimd.html>. There is no product yet, but the technology is covered under US patent 4922467. Could not find open literature references.

A variety of IMS scanners and portals have been produced by Barringer (recently bought out by Smith Detection). The IONSCAN® Model 400B is extremely sensitive, has a very low false alarm rate and completes an analysis in 6-8 seconds. The SABRE 2000 is the only hand held detector capable of detecting drugs, explosives, chemical warfare agents and toxic industrial chemicals. The IONSCAN® SENTINEL II is a non contact portal that screens people for traces of explosives and narcotics, quickly and accurately, without coming into contact with them. The COMPASS Body-Scanner is the ultimate body scanner for detecting passengers carrying metal and non metal weapons, explosives, dangerous liquids, diamonds, gold and illicit drugs (including those swallowed).

Another company that has developed an advanced passenger screening technology is Rapiscan whose Secure 1000 x-ray technology gives a front and back body scan in five seconds.

A system using TNA technology is the Small Parcel Explosive Detection System (SPEDS) from Ancore. It detects explosives in hand-carried items such as portable electronics, briefcases, mobile phones, small handbags, bottles of liquid, etc. Small or medium size postal packages, large enough to contain pipe bombs or more sophisticated explosives, can also be inspected by the SPEDS. The system is especially sensitive to liquid explosives.

Spatial Dynamics of Clarkston, Washington assembled and calibrated their first prototype passenger screening system at the FAA William J. Hughes' Security Operations Center (SOC) in Atlantic City, NJ. Studies are being initiated to evaluate safety, health, and human factors to support a petition to the FAA's Institutional Review Board for authority to conduct limited lab detection testing. This prototype, currently referred to as the "Dielectric Portal" developed under FAA sponsorship, uses extremely low power microwaves to measure subtle differences in body dielectric properties in order to detect concealed explosives and weapons. The Dielectric Portal displays a standard stick figure for indicating the presence and location of potential threat objects. Based on initial measurements, the total scan process and display time, is less than 4 seconds per person and offers nearly 100% scan coverage.

3.2 Luggage Screening

Most of the bulk explosives detection equipment that has been deployed or is being considered for deployment is X-ray based – the exception being the InVision/Quantum Magnetics Q-Scan, which is based on a nuclear quadrupole resonance measurement technique. The X-ray based technologies that have been deployed or scheduled for deployment include transmission, dual energy, and CT. Of these, only the CT system has been FAA certified.

The Tables below show the deployment statistics for explosives detection equipment as of 1999 (Data from the National Academies 1999 report):

TABLE 6-2 Location of Deployed Bulk Explosives-Detection Equipment (April 1999)

Location	InVision CTX	Vivid VIS-1	EG&G Z-scan 7	Heimann HI-Scan	InVision/QM Q-Scan	Total
Lobby stand-alone	40	1				41
Lobby/curbside integrated ^a	19	1		2	1	23
Bag room, stand-alone	3					3
Bag room, integrated ^a	12		4			16
FAA Technical Center	1					1
To be determined		6	6		1	13
Totals	75	8	10	2	2	97

^a Screening device is either partially or fully integrated into airline baggage-handling system.

TABLE 7-2 Status of TEDD Deployment (as of January 31, 1999)

Manufacturer	Model	Number Deployed	Number to Be Deployed in FY 1999	Total
Barringer	Ionscan 400	178	220	398
Ion Track	Itemizer	80		80
Thermedics	Egis 3000	55		55
	Egis 2	—	5	5
IDS	Orion	53		53
To be determined			40	40
Total		366	265	631

Of course, since 2001 the number of installed systems has skyrocketed, but actual installation numbers are difficult to find.

The largest producer of these devices is InVision Technologies, with several on the market:

FAA certified detection systems for explosives.

CTX9000CSI x-ray imaging and CT scan luggage portal

CTX5500DS same as above, lower throughput, trainer available

CTX2500 same as above, smaller footprint

Qscan QR500 Quadrupole Resonance

Qscan QR160 same as above, smaller

i-Portal 100 Weapons Detection Systems using electromagnetic anomaly detection technology

Cargo containers and trucks can be inspected quickly, automatically, and non-intrusively with Ancore's Pulsed Fast Neutron Analysis (PFNA) technique. PFNA determines the elemental contents within small volume segments of a scanned object. These measurements are used to generate three-dimensional maps of the cargo's elemental composition. Specific substances and contraband then can be identified using the PFNA's imaging system, as the images provided by PFNA display the position and extent of contraband in the cargo container or truck. The entire process is fully automated and does not rely upon human operator interpretation. PFNA thereby is virtually immune to concealment.

Ancore's Cargo Inspector (ACI), is based on the PFNA technology, is automatic and highly effective. The ACI detects a wide range of contraband including explosives, narcotics, hazardous chemicals, chemical agents and other weapons of mass destruction (such as radiological or nuclear) and their components, and many specific dutiable goods, etc.

The Mobile Vehicle and Cargo Inspection System (VACIS) is a truck-mounted gamma-ray imaging system designed to non-intrusively inspect the contents of trucks, containers, cargo and passenger vehicles for explosive devices and/or contraband ...

The Fixed Vehicle and Cargo Inspection System (VACIS) is a new technology for non-invasive imaging of trucks, sea containers, and other vehicles which may contain contraband, miss-manifested cargo, explosives or weapons...□

Railroad Inspection System is designed to inspect railroad cars as they pass through a specified inspection area...

In the fourth quarter of FY2000, L-3 won additional funding to develop the 3DXTM 3000, a smaller-scale version of its Federal Aviation Agency- certified eXaminer 3DX 6000, currently being used in domestic and international airports. In January of 2001, L-3 received an order from the FAA for six additional eXaminer 3DX 6000 systems, and also received FAA certification for the 3DX 3000. "With this new product," said Lanza, "we have a significant advantage over our competition because we can offer the most advanced products for both large and smaller airports."

Analogic Corporation (NASDAQ: ALOG), a leading manufacturer of high precision medical and industrial, diagnostic and measurement instruments and equipment, announced today it had been notified by the Federal Aviation Administration (FAA) that L-3/Analogic's " eXaminer 3DX 6000™ " explosive detection system (EDS), an airport security system that detects a wide range of explosive devices in airline passenger baggage, had been granted certification by that agency. The eXaminer 3DX 6000, which incorporates the Analogic state of the art EXACT™ CT machine as well as detection algorithms for sheet-like forms of explosive also developed by Analogic, is capable of generating three-dimensional images of all objects in bags and is the only single-unit, second-generation system presently certified by the FAA.

The CT portion of the system is the result of a technical proposal prepared by Analogic for presentation to the FAA in response to their requirement for a new generation of economical faster, and more accurate and reliable systems. The development of the CT portion of the system was completed by Analogic in record time.

The EDS exceeds the FAA's stringent requirements for identification of difficult-to-detect plastic explosives in passenger baggage and for rapid bag throughput with a low false alarm rate. With eXaminer capabilities superior to existing first-generation systems, it is the first EDS to provide multiple, simultaneous and continuous computed tomography (CT) images to examine an entire bag in one pass, analyzing 10 times more data per bag than the existing generation of machines. Using Excalibur accelerators from SKY Computers, the new system has been certified to process 500 bags per hour, more than twice the capacity of existing systems. The eXaminer 3DX 6000 is also approximately half the size and weight of first-generation explosive detection systems, a key feature given limited airport space.

Galaxy Scientific Corporation adapted a novel image analysis method to CT machines used in explosives detection and has created a visual basic program to carry out this complicated analysis of image quality automatically. The method consists of passing a thin, precisely machined, circular plastic disk, called a "phantom," having a uniform density, through the CT machine and capturing the reconstructed image. The image is then analyzed for resolution and noise content.

To characterize the machine's resolution the change of the CT numbers across the edge of the phantom image is measured. The result of this measurement is called the edge response function (ERF). The first spatial derivative of the ERF is then calculated which gives the point spread function (PSF). The Fourier transform of the PSF results in the modulation transfer function (MTF). The MTF is what quantitatively gives a measure of the resolution of the system. Galaxy's analysis program generates and plots these three measures of image resolution directly from the stored reconstructed phantom image.

The noise level of the image is characterized by the contrast discrimination function (CDF). Galaxy's analysis program, following ASTM recommendations, divides the phantom image into multiple square areas. It then calculates the standard deviation of the CT numbers within each square, finds the average standard deviation, and multiplies that result by three. This provides one data point for the CDF curve. The area of the squares is increased and the process is repeated to provide the next data point. This procedure continues until the specified maximum area of squares is reached. The collection of these data points constitutes the CDF. The ASTM standard specifies that if the CT numbers of an object in an image are greater than three times the standard deviation of the CT numbers in the image, then the object is distinguishable from the background noise.

Galaxy has also expanded the image analysis process outside of what the ASTM standard requires. The Galaxy analysis program plots the change in CT number at four angles from the edge of the field of view, through the center of the phantom image, to the opposite edge. The program also plots the change in CT number at the same four angles through the center of the field of view. These plots help to uncover and quantify ring artifacts in the reconstructed image. These ring artifacts are due to x-ray detectors that are out of calibration.

3.3 Testing Materials and Methodology

An FAA certified EDS is a self-contained unit (composed of one or more integrated devices) that has passed the FAA certification test, which is: the detection rates against various types of explosives contained in baggage must have an overall probability of detection of no less than X (classified number, see FAA 1992)). The probability of false alarm (as determined for airline type baggage) must not exceed Y (classified number). The baggage throughput must meet or exceed 450 bags / h. (Source: *Federal Aviation Administration. 1992. Proposed Criteria for Certification of Explosives Detection Systems as Defined under 14 CFR 108.20. Washington, D.C.: Federal Aviation Administration.*

The Threat Image Projection Library (FAA Transportation Security Laboratory) provides a means to randomly insert threat images into passenger bags as they pass through airport checkpoints. It is then the responsibility of the screener to identify the potential threat and take appropriate actions.

The Threat Image Projection Library consists of 2400 images and is intended to provide x-ray images of past, current, and potential threats to the airline industry. In developing these images,

first-hand knowledge and comprehensive research into current trends of terrorist organizations worldwide was essential, as was a certain amount of ingenuity, because many of the devices used by terrorist organizations integrate stuffed animals, toys, and electronics with detonators, explosives, and switches to create a deadly and unseen threat.

The overall objective of an interagency agreement between the FAA and the INEEL is to provide the FAA with the necessary information to meet its mission of assuring air passenger safety. Under the proposed tasks, the INEEL will support this mission by: 1) providing additional information about the levels of particulate explosives and volatile taggants emitted from explosives in luggage; 2) supporting the FAA mission through the necessary program management, consultation, facilities, and equipment support; 3) quantifying explosive on suitcase material; 4) quantifying explosive on personnel clothing; and 5) quantifying explosive on personal identification materials (passports, boarding passes).

Methodology/human subject involvement: The contractor (INEEL) will quantify the amount of explosive deposited on the surfaces of clothing material worn by improved explosive device manufactures. The types of explosives to be tested are Composition C-4, Detasheet, Semtex-H, Trinitrotoluene (TNT), and nitroglycerine dynamite, and a smokeless propellant. During testing, the participant may be instructed to (1) place their thumb and fingers on a small block of explosive material and press down at prescribed pressures, (2) use the fingerprints to transfer the particles onto other materials (such as paper or cardboard), and/or (3) manipulate an explosive in a manner that roughly simulates the making of an explosive device (e.g. unwrap explosive, place into containers or other configurations, re-wrap explosive).

In DT&E, Galaxy plans, designs, and conducts tests; analyzes test data; and prepares test reports. Galaxy also supports testing on breadboard units, subsystems, and system levels at vendor facilities and field prototype testing. The support includes test design and test protocol development, test bag selection and documentation, test article preparation and documentation, test conduct, simulant validation, test data analysis, documentation of test results, revision of standard operating procedures, software and database support, and database development.

Galaxy has tested and evaluated the following EDDs/EDSs: L3 eXaminer 3DX 6000, InVision CTX 5500 DS, InVision 9000 Galileo, InVision CTX 2500, L3 Vivid MVT, QM 60, QM 160, Heimann 10065, 3 Systems (Vivid/EG&G/Heimann), 4 Systems Operator Assist Carry-On (EG&G/RapiScan/Vivid/Heimann), 2 Systems Data Collection (RapiScan/NQR), Vivid VIS-M, as well as the 2 Systems (EG&G Z-Scan 7/Vivid VIS-M), Magal AISYS Detonator Detection Device, Spatial Dynamics Passenger Portal, QM SuperScan 450, Aeye/EG&G Detonator Detection Software, and all trace EDDs. The technologies associated with the EDDs/EDSs include x-ray/computer tomography detection, neutron detection, nuclear backscatter, nuclear magnetic resonance, dielectric constant, gas chromatography, chemiluminescence, and ion mobility spectrometry.

Galaxy Scientific Corporation's explosives specialists use real world knowledge and experience to design and construct state-of-the-art improvised explosive devices (IEDs). Galaxy has used this capability to develop a Threat Image Projection Library, which is being used by the Federal Aviation Administration and the Governments of Israel, Great Britain, Canada, and France.

The Galaxy Image Quality Test Kit, consisting of a Lucite phantom and the analysis program, can be used to establish an image quality baseline for a given CT machine, which can then be compared to subsequent analyses conducted over time to evaluate any change in image quality. The discovery of degradation in image quality is construed as a signal of possible hardware problems that need correction.

Galaxy plans, designs, and conducts tests and analyzes test data of explosives detection devices (EDDs)/explosives detection systems (EDSs). Testing evaluates system performance against FAA performance standards and includes validation of vendor data package and conduct of formal tests in a realistic environment. Tasks include standardizing test bag sets, validating simulants, selecting test bags, developing test designs and test protocols, preparing test articles, conducting tests, and documenting test results.

3.4 Other Testing Technologies

Mistral

Red Dot Expray color reaction test kit for the detection and identification of Group A explosives (e.g. TNT, TNB, etc.), Group B explosives (e.g. Semtex H, RDX, C4, etc.) and compounds containing inorganic nitrates that are used in improvised explosives (e.g. ANFO).

Detection Chart

Product : EXPRAY -1			EXPRAY - 2		EXPRAY - 3	
Detects: Polynitro Aromatics			Nitrate-esters Nitramines		Inorganic Nitrates	
Group A			Group B		Group C	
#	Substance	Color	Substance	Color	Substance	Color
1	TNT	Dark Brown	Semtex	Pink	Ammonium Nitrate	Pink
2	TNB	Dark Brown	RDX	Pink	Potassium Nitrate	Pink
3	DNT	Blue Green	HMX	Pink	Sodium Nitrate	Pink
4	Picric Acid	Yellow	PETN	Pink	Barium Nitrate	Pink
5	Tri Nitro Napthalene	Violet	EGDN	Pink	BlackPowder	Pink
6	Lead Styphnate	Yellow	Nitro Glycerin	Pink		
7			Nitro Cellulose	Pink		
8			Tetryl	Pink		
9			Smokeless Powder	Pink		

TABLE 7-1 Most Effective Techniques for Sampling Explosives for TEDDs

Explosive	Technique
RDX	Wiping
PETN	Wiping
TNT	Wiping
EGDN	Vapor detection
OMNT	Vapor detection
PMNT	Vapor detection
DMNB	Vapor detection
NG	None known

Swiping methods are used routinely to survey baggage, especially carry-on baggage. The protocol usually used is illustrated in the figure below:

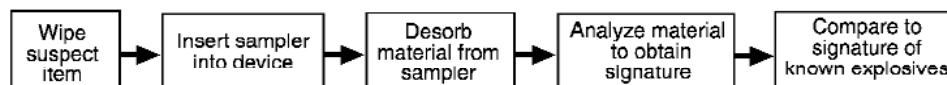


FIGURE 7-1 Operational steps of a trace explosives-detection device.

The swipes are analyzed using IMS or GC/IMS in presently installed equipment, such as the Barringer IONSCAN® Model 400B, which is extremely sensitive, has a very low false alarm rate and completes an analysis in 6-8 seconds, or the GC/Ionscan, which couples a short column GC for additional selectivity and reduced false alarm rate.

The GC-IONSCAN® is a trace detector that gives the user the option of fast, accurate IMS detection ideal for pre-screening, or the more detailed analysis of a sample using gas chromatography while benefiting from the identification power of IMS detection (GC-IMS).

3.5 Web Site References:

<http://api.hq.faa.gov/sp01/sp2001.html>
<http://www.tc.faa.gov/aar500/content/aar520.asp>
<http://books.nap.edu/books/0309067871/html/index.html>
<http://www.airport-technology.com/contractors/security/index.html>
<http://www.analogic.com/Level3/Newsreleases/1998%20newsreleases/Bombscanner.html>
<http://www.ancore.com/products.htm>
<http://www.ancore.com/speds.htm>
<http://www.as-e.com/products/products.html>
<http://www.dsxray.com/products.asp>
<http://www.eml.doe.gov/hsrd/hsr00/INEEL.htm>
<http://www.eurotechltd.com/products/nets/acimd.html>
<http://www.galaxyscientific.com/areas/securtech/securtechindex.htm>
<http://www.galaxyscientific.com/areas/securtech/simied.htm>
<http://www.invision-tech.com/products/products.htm>
<http://www.lcairport.net/portal.htm>
<http://www.mistraldetection.com/expray.htm>
<http://www.smithsdetection.com/Products/>
<http://www.rapiscan.com/>